# **I-V Characteristics Calculation Using SCAPS-1D Program**

# SCAPS-1D Programı Kullanılarak I-V Karakteristiklerinin Hesaplanması

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## Özet

Bu çalışmada, güneş pili modellemesi için en yaygın kullanılan simülasyon yazılımlarından birini sunuyoruz. SCAPS-1D programının kullanımı bu çalışmada adım adım anlatılmıştır. İlk adımda, heteroeklem güneş pillerini sunduk ve fotovoltaik etkiyi açıkladık. SCAPS programının işleyişini açıklamak için, bu programın kısa bir tarihçesiyle başladık ve ardından farklı özelliklerinin genel bir tanımıyla devam ettik. Bu programı çalıştırmak ve bir güneş pilinin I-V özelliklerini elde etmek için gereken tüm bu adımları önceden tanımlanmış bir örnek aracılığıyla netleştirdik. Sonunda, CdS/CIGS heteroeklemli güneş pili üzerindeki V<sub>oc</sub> ve J<sub>sc</sub> üzerindeki optik bant aralığı değişiminin örnek bir çalışmasını yaptık.

Anahtar kelimeler: SCAPS\_1D, Güneş Hücresi, İnce Filmler, CIGS

## Abstract

In this work, we present one of the mostly used simulation software for solar cells modelling. The usage of SCAPS-1D program has been explained in this work step by step. At the first step, we have presented the heterojunction solar cells and explain the photovoltaic effect. To elucidate SCAPS program operation, we have started by a brief history of this program and then continued with a general definition of its different properties. By the mean of a predefined example, we have clarified all the stages needed to operate this program and to obtain I-V characteristics of a solar cell. At the end, we have made an example study of optical band gap variation on the  $V_{oc}$  and  $J_{sc}$  on CdS/CIGS heterojunction solar cell.

Keywords: SCAPS\_1D, Solar Cells, Thin Films, CIGS

#### 1. Introduction

The direct conversion of incident light photons energy into electric energy by a p-n semiconductor junction device has been known as the photovoltaic (PV) effect. When Chapin *et al.*[1] has presented the silicon solar cells with a 6% conversion rate in 1954, it was considered as the initiation of a new era of PVs. This phenomenon had already been known for over a century. In that concept, solar cells have been quickly considered as a very effective way of continuously powering remote location devices, especially for the space industry. Of course, this application of photovoltaic spread rapidly to other uses that exist in our daily life. The structure, properties and operation principles of solar cells have been thoroughly studied worldwide and reported in literature [2]. When photon energy is larger than or matches the energy bandgap of semiconductor in use, they can be absorbed by the material. The gained energy as a result of absorption of photon excites electron from the valance band to the conduction band where it can freely move leaving behind a hole (absence of electron). When the generation of the electron- hole pair is in the depletion region (the contact area in the p-n junction of solar cell), the existing field in this area will separate them where they can be collected at the exterior (left and wright) contacts.

Even though the concept of the solar cells is simple, but its construction and development consume lots of time and energy. In order to overcome this problem, some groups have started developing various programmes and worked on modelling of these solar cells. The complexity level of the programs changes from one to another and it mostly depends on the introduced output data. The most common used programs in the recent years are COMSOL [3], SILVACO ATLAS [4], AMPS [5], wxAMPS [6], and SCAPS [7-12]. Among these software SCAPS program is considered to be very easy for beginners with very vast range of output and input data [7]. In this article, we have intended to introduce this program and give a brief explanation on its multiple functions.

#### 2. Heterojunction Solar Cells

In order to understand SCAPS program better, we will start by introducing what is a solar cell first and then what are its different electric parameters?

An n-type window layer, a p-type absorber layer and a junction between them make up a conventional window-absorber p-n type junction solar cell as present in Fig.1. In a homojunction device, these areas are made of the same material, but in a heterojunction device, they are made of two distinct materials.

The junction between p- and n-type regions is considered as the most essential part of any solar cell. In this region, the charge separation of holes and electrons is taken place by absorption of energetic photons at the charge depletion region. Hence, it plays a big influence in determining device performance. When performance of a solar cells is studied, four different parameters are observed; efficiency ( $\eta$ ), the short circuit current (J<sub>sc</sub>), fill factor (FF) and the open circuit voltage (V<sub>oc</sub>).



Figure 1: A schematic image of a pn junction solar cell.

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#### 3. SCAPS-1D definition

The first version of SCAPS-1D program was developed in 1998 by Marc Burgelman group at the university of Gent, Department of Electronics, and Information Systems (ELIS), Belgium. After that more than 50 versions has been developed until late this year (SCAPS 3.3.10) [13, 14]. This software is freely available with an easy working interface where the user can manipulate the different solar cells input parameters such as the thicknesses of different layers, the doping concentration, some electric properties such as mobility and dielectric effect, the doping distribution and concentration, the contacts different properties, etc. On the other hand, the usual calculated outputs using this program are I-V, C-V, C-f, QE. In order to use SCAPS-1D software correctly, some important steps must be taken into consideration. The example presented in this explanation section is taken from the SCAPS-1D package.

#### **3.1.** Opening and Loading

On the Desktop or on the file manager open the program or the scaps3310.exe file. The opened window is SCAPS Action Panel (Fig.2), on the left, click on the "Set problem" button and then choose "load" on the lower right of the Solar Cell Definition Panel. From the previously defined solar cells, we will choose "example CIGS.def" file and load it (Fig.3).

<ul> <li>SCAPS 3.3.10 Action Panel</li> </ul>							- 🗆 X
Working point Temperature (K)	Series res	istance —— es	—Shunt resistand	xe A	ction list	· /	All SCAPS settings -
Voltage (V) 20.0000		D	no	Loa	d Action Li	st	Load all settings
Frequency (Hz) = 1.000E+6 Number of points = 5	<u>≜1.00E+0</u>	Rs Ohm.cm <sup>°</sup> S/cm <sup>°</sup>	2 Rsh 1.00E+ 2 Gsh 1.00E-3	3 3 3	ve Action Li	st	Save all settings
Illumination: Dark Lig	ht Speci	fy illumination sp	ectrum, then calculate (	G(x) Directly :	specify G(x	)	
Analytical model for spectrum Spectrum file name: illumir	ated from left	ated from right	Incident (or b light power (W	pias) /m2)	ytical mode	I for G(x)	G(x) from file
Select	AM1_5	G1 sun.spe	sun or lamp 0.00	G(x) mode	el [	Constant gene	eration G
Spectrum cut off?	Shortwavel. (nm) 20	0.0	after cut-off 0.00	Ideal Transi		nt in G(x) (mA attenuation filt	/cm2) 20.0000 er(%) 100.00
Neutral Density 0.0000	Transmission (%)	0.000	after ND 0.00	Idea	Light Curre	ent in cell (mA	/cm2) 0.0000
Action -Pau	se at each step				number -		
F I-V	V1 (V) 🛱 0.0000	V2 (V)	0.8000		<b>4</b> 1	\$ 0.0200	increment (V)
□ C-V	V1 (V) 🖨 -0.8000	V2 (V)	0.8000		\$81	0.0200	increment (V)
C-f	f1 (Hz) 🚔 1.000E+2	f2 (Hz)	1.000E+6		21	5	points per decade
C QE (IPCE)	WL1 (nm) 🚔 300.00	WL2 (nm)	900.00		<b>\$</b> 61	\$ 10.00	increment (nm)
Set problem	loaded definition file:			Problem file: ne	ew problem	Set Prob	lem
Calculate: single shot	Continue	Stop	Results of	of calculations		Sa	ve all simulations
Calculate: batch	Batch set-up	E	B G,R AC	I-V C-V C	f QE	Cle	ar all simulations
Calculate: recorder	Record set-up		Recor	rder results		j	SCAPS info
Calculate: curve fitting	Curve fit set-up		Curvef	itting results		J	
Execute script	Script set-up		Script graphs	Script var	iables	]	Quit

Figure 2: Action Panel in SCAPS program.

SCAPS 3.3.10 Solar Cell Definition Panel						-		×
Layers		illuminated from : apply voltage V to : right   left contact		current reference as a:		Invert the structure		
left contact (back)				gonoration	_			
CIGS	Interfaces							
OVC -								
CdS -	OVC / Cas							
i-ZnO						*		
add layer —						-		
						*		
		, <b>.</b>						
right contact (front)		left con	loci	rigt	hi contact			
******		back		fro	n	-		
Info on graded parameters only available	after a calculation	<u> </u>						
Problem file numerical set	tings							
c:\Program Files (x86)\Scaps3309\def\ example CIGS.def last saved: 1-9-2015 at 13:44:6								
Remarks (edit here)								
SCAPS 3.3.02 ELIS-UGent Version scaps last saved by SCAPS: 01-09-2015 at 13:44	3302.exe, dated 28-08-2015, 1 :04	11:48:47 Problem c <sup>_1</sup>		new	load		save	
This problem definition file has been distri Here this old def file is saved in the format	buted with all SCAPS version: now used by SCAPS2.8	s since SCAPS 2.0		cancel			ОК	

Figure 3: Solar Cell Definition Panel in SCAPS program.

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#### 3.2. Definition of Solar Cell

In our case, the different layers are already defined in a conventional p-n heterojunction solar cell. Thus, we will clarify the different chosen parameters of p-type CIGS absorber layer as an example by clicking on the layer button (Fig.4).

On the right of the "Layer Properties Panel", we can fill out the different electric properties of the layer such as the optical band gap, the dielectric permittivity, the electron affinity, electron/hole mobility and the thickness as well. Down to the right, the absorption of the material can be set from a model or from the previously available files in the absorption library of the program. The defect on the left side of this panel is divided into three different types: Auger and radiative recombination which present band to band transition, also the SRH (Shockley-Read-Hall) recombination. In this model, they set only the SRH recombination by introducing a neutral, single, and uniform defect level with a defect density of 10\*E18. After setting all the various properties of a layer, we can save the changing by clicking on "Accept" button. On both sides (up and down) of the structure on the right, we can also change the properties of the back and front contacts and also define a specific defect density at the interfaces between the different layers.

SCAPS 3.3.10 Layer Properties Panel					-	
LAYER 1		CIGS	Recombination model			
thickness (μm) 💌	1.000		Band to band recombination			
	uniform pure A (y=	0) -	Radiative recombination coefficient (cm³/s)	0.000E+0		
The layer is pure A: y = 0, uniform	0.000		Auger electron capture coefficient (cm^6/s)	0.000E+0		
Semiconductor Property P of the pure material	pure A (y = 0)		Auger hole capture coefficient (cm^6/s)	0.000E+0		
			Recombination at defects: Summary			
bandgap (eV)	1.200		Defect 1			
electron affinity (eV)	4.500		Defect 1			
dielectric permittivity (relative)	10.000		charge type : neutral			
CB effective density of states (1/cm^3)	2.000E+18		total density (1/cm3): Uniform 1.000e+18 grading Nt(x): uniform			
VB effective density of states (1/cm^3)	2.000E+18		energydistribution: single: Et = 0.60 eV above E'	v		
electron thermal velocity (cm/s)	1.000E+7		this defect only, if active: tau_n = 1.0e-01 ns, tau_p = 1.0e-01 ns			
hole thermal velocity (cm/s)	1.000E+7		this defect only, if active: Ln = 1.1e-01 µm, Lp = 3	7.2e-02 μm		
electron mobility (cm²/Vs)	5.000E+1					
hole mobility (cm²/Vs)	2.000E+1					
effective mass of electrons	1.000E+0					
effective mass of holes	1.000E+0					
no ND grading (uniform)		-				
shallow uniform donor density ND (1/cm3)	0.000E+0					
no NA grading (uniform)		-				
shallow uniform acceptor density NA (1/cm3)	5.500E+15					
Absorption interpolation model						
alpha pure A material (y=0)	how					
from file 🔲 from model	now		Edit Add a			
Set absorption model	ave		Defect 1 Defect 2			
List of absorption submodels present			Bemove			
sqrt(hv·Eg) law (SCAPS traditional)						
			(no metastable configuration possible)			
			Accept cancel Load	Material Save Materia		

Figure 4: Layer Properties Panel in SCAPS program.

#### **3.3.** Operating of the program

After completing the simulation model of the solar cell, it is time to start testing the program by clicking on "OK" button that will take us back to the Action Panel.

At the upper left of the "Action panel", we can define the working points that will be constant during the calculation process such as the temperature, the voltage, and the frequency. During the illumination mode, different types of spectrums can be defined according to the solar cell type and the wanted wavelength range that the solar cell will be working under.

In our case, we want to calculate I-V characteristics of the predefined solar cell so we will choose I-V checkbox. When the calculation ends, we can see the results by clicking the I-button on the right to open the I-V Panel as present in Fig.05. The I-V graph and the I-V characteristics like  $V_{oc}$  and  $J_{sc}$  can be seen at the interface, and we can also save them by clicking on "Save" button.

To study the effect of a certain properties like the thickness on the  $V_{oc}$  we can change this property using the "Bach set-up" Button (Fig.2) and then applying on "calculate Bach" button.



Figure 5: The I-V Panel in SCAPS program.

## 3.4. Example on the effect of absorber layer band gab variation

In this case, we will change the optical band gap values of the CIGS absorber layer from 0.9 eV to 1.6 eV and observe its effect on the  $V_{oc}$  and  $J_{sc}$  of the solar cell. In Fig. 6, the band gap increasing resulted in changing the values of  $V_{oc}$  from 0.3 eV to 0.9 eV. Thus, we can see that the program can detect the altering of the solar cells parameters and show its influence on the output data. Also in Fig.7, we can see that contrary to the  $V_{oc}$ ,  $J_{sc}$  values decreased by augmenting the band gap where it reduces from 43.4 mA/cm<sup>2</sup> to 19mA/cm<sup>2</sup>, these observation are well explained in many article [15].



Figure 6: Simulated Voc with increasing band gap values

Figure 7: Simulated Jsc with increasing band gap values

### 4. Conclusion

In this article, we have given a brief introduction on the well-known SCAPS-1D simulation program used to simulate and predict the performance of the different solar cells. We have also provided explanations on the general use of this software. In addition, by using an existed model on the program library, we have

described the general steps that must be followed to successfully obtain correct results on this program. At the end, we have presented an example study of the bag gap variation on the optoelectrical outputs of a solar cell.

### 5. References

- [1] D. M. Chapin, C. S. Fuller, and G. L. Pearson, "A new silicon p- n junction photocell for converting solar radiation into electrical power," *Journal of Applied Physics*, vol. 25, no. 5, pp. 676-677, 1954.
- [2] L. M. Fraas and L. D. Partain, *Solar cells and their applications*. John Wiley & Sons, 2010.
- [3] S. Zandi, P. Saxena, and N. E. Gorji, "Numerical simulation of heat distribution in RGO-contacted perovskite solar cells using COMSOL," *Solar Energy*, vol. 197, pp. 105-110, 2020.
- [4] A. Hima, N. Lakhdar, B. Benhaoua, A. Saadoune, I. Kemerchou, and F. Rogti, "An optimized perovskite solar cell designs for high conversion efficiency," *Superlattices and Microstructures*, vol. 129, pp. 240-246, 2019.
- [5] Y. Hamri *et al.*, "Improved efficiency of Cu (In, Ga) Se2 thinfilm solar cells using a buffer layer alternative to CdS," *Solar Energy*, vol. 178, pp. 150-156, 2019.
- [6] A. Bag, R. Radhakrishnan, R. Nekovei, and R. Jeyakumar, "Effect of absorber layer, hole transport layer thicknesses, and its doping density on the performance of perovskite solar cells by device simulation," *Solar Energy*, vol. 196, pp. 177-182, 2020.
- [7] A. Houimi, S. Y. Gezgin, B. Mercimek, and H. Ş. Kılıç, "Numerical analysis of CZTS/n-Si solar cells using SCAPS-1D. A comparative study between experimental and calculated outputs," *Optical Materials*, vol. 121, p. 111544, 2021.
- [8] J. Wang *et al.*, "Simple Solution- Processed Approach for Nanoscale Coverage of Perovskite on Textured Silicon Surface Enabling Highly Efficient Perovskite/Si Tandem Solar Cells," *Energy Technology*, vol. 9, no. 1, p. 2000778, 2021.
- [9] M. A. Ashraf and I. Alam, "Numerical simulation of CIGS, CISSe and CZTS-based solar cells with In2S3 as buffer layer and Au as back contact using SCAPS 1D," *Engineering Research Express*, vol. 2, no. 3, p. 035015, 2020.
- [10] D. Dwivedi, "Numerical simulation for enhancement of the output performance of CZTS based thin film photovoltaic cell," *Advanced Science, Engineering and Medicine*, vol. 12, no. 1, pp. 88-94, 2020.
- [11] H. Shen *et al.*, "Monolithic perovskite/Si tandem solar cells: pathways to over 30% efficiency," *Advanced Energy Materials*, vol. 10, no. 13, p. 1902840, 2020.
- [12] S. Tripathi, P. Lohia, and D. Dwivedi, "Contribution to sustainable and environmental friendly non-toxic CZTS solar cell with an innovative hybrid buffer layer," *Solar Energy*, vol. 204, pp. 748-760, 2020.
- [13] M. Burgelman, K. Decock, A. Niemegeers, J. Verschraegen, and S. Degrave, "SCAPS manual," ed: February, 2016.
- [14] M. Burgelman, K. Decock, S. Khelifi, and A. Abass, "Advanced electrical simulation of thin film solar cells," *Thin Solid Films*, vol. 535, pp. 296-301, 2013.
- [15] J. Jiang *et al.*, "Optimization bandgap gradation structure simulation of Cu2Sn1- xGexS3 solar cells by SCAPS," *Solar Energy*, vol. 194, pp. 986-994, 2019.