

SLALOM: Open-Source, Portable and Easy-to-use Solar Cell Optimizer. Application to the Design of InGaN and CZTS Solar Cells.

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Summary





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SLALOM: Open-Source, Portable and Easy-to-use Solar Cell Optimizer. Application to the Design of InGaN and CZTS Solar Cells. Sidi OULD SAAD HAMADY ^(1,2,*), Nicolas FRESSENGEAS ^(1,2) ¹ Université de Lorraine, Laboratoire Matériaux Optiques, Photonique et Systèmes, Metz, F-57070, France ² Laboratoire Matériaux Optiques, Photonique et Systèmes, CentraleSupélec, Université Paris-Saclay, Metz, F-57070, France * sidi.hamady@univ-lorraine.fr

The development of new thin films solar cells is highly accelerated by using rigorous optimization approach. A large set of parameters is involved in the solar cell operation: active layer thickness, composition, bandgap, doping, contacts, etc. The study of the solar cell performances with respect to these linked parameters is necessary to better understand the underlying physics and to optimize the final device. We propose in this poster presentation (*) a new open-source solar cell optimizer: SLALOM for SoLAr cell multivariate OptiMizer. SLALOM implements, for the first time for solar cells, a rigorous multivariate approach while the standard optimization work used to use the one-by-one parameter procedure. SLALOM is implemented to be easily extended to any simulator, the core code itself does not depend on any particular engine. It can be adapted for any solar cell structure, runs locally or remotely on a calculation server, using the SSH protocol and includes a graphical user interface to real-time monitor the optimization. Two study cases, InGaN and CZTS solar cells, are presented to show the SLALOM ability to become a useful tool for the development of novel solar cells. (*) Article independently submitted to EPJ Photovoltaics

SLALOM: principle, implementation and application to InGaN and CZTS solar cells

CLASSICAL OPTIMIZATION METHOD: THE PARAMETRIC ANALYSIS



One-by-one parametric analysis steps (cf. figure):

- \rightarrow defining a set of technological and physical parameters: composition, doping concentrations, layers thicknesses...
- \rightarrow defining the set of samples to simulate
- \rightarrow simulating these samples to extract the photovoltaic efficiency

The sample for which the efficiency is optimal in then identified and the varying parameter set to the optimal value. The procedure then iterates for the next parameter, keeping all other parameters constant...

Advantage:

 \rightarrow simplicity

Disadvantages:

 \rightarrow mathematical uncertainty: at the end of the procedure, the highest obtained efficiency is not guaranteed to be the optimal one since the procedure ignores the interdependence between the solar cell parameters

SLALOM: RIGOROUS OPTIMIZATION METHOD

SLALOM (SoLAr cell multivariate OptiMizer):

- \rightarrow uses state-of-the-art mathematical optimization algorithms to find the parameter set that yields the optimal solar cell efficiency
- \rightarrow takes the interdependence between the parameters into account
- \rightarrow minimizes the computing time, if compared to the classical method **Procedure steps:**
- \rightarrow defining a set of parameters pertaining to the solar cell operation (e.g. composition, doping concentrations, layers thicknesses...)
- \rightarrow using a semiconductor simulation engine that allows the numerical evaluation of the solar cell efficiency from its parameters (cf. figure) \rightarrow using a mathematical algorithm designed to find the parameter vector that maximizes the efficiency using a numerical iterative
 - procedure



- **Used mathematical optimization algorithms:**
- \rightarrow Sequential Least Squares Programming (SLSQP) method: starting from an initial guess, it uses Newton's method to find the optimum \rightarrow Broyden–Fletcher–Goldfarb–Shanno (BFGS) iterative algorithm: it
- uses a quasi-Newton method to find the optimum using gradient

SLALOM: IMPLEMENTATION



SLALOM is written in Python, It uses the SciPy and NumPy numerical packages, Tkinter for the user interface and Matplotlib for 2D curve plotting. Figures shows the SLALOM general architecture.

SLALOM modules:

- \rightarrow slalom.py: the SLALOM startup module: sets the parameters, the optimization method and controls the whole process
- \rightarrow slalomCore.py: the SLALOM core class: implements the optimization using mathematical algorithms and controls the device simulation engine
- \rightarrow slalomDevice.py is a class defining a set of devices (e.g. InGaN PN, CZTS NP...) for easier and more robust optimization work
- \rightarrow slalomDeviceGui.py is a class providing an interface to create a new device type

SLALOM is distributed under MIT license for free use, modification and redistribution. Its source code is freely available for download and use from: \rightarrow https://github.com/sidihamady/SLALOM

APPLICATION TO INGAN AND CZTS SOLAR CELLS





- \rightarrow Illumination : 1 Sun with AM 1.5G Solar Spectrum.
- \rightarrow InGaN Bandgap, Affinity, Effective density of states, Permittivity, Absorption, SRH, Auger and direct recombination, Band discontinuity, Tunneling **Polarization/Piezoelectric** current,



Efficiency of the InGaN PN solar cell determined by SLALOM using the L-BFGS-B and SLSQP methods: both methods converge to the same set of optimal parameters in about two hours for L-BFGS-B and one hour for SLSQP on a Red Hat Linux server with two 8-core Xeon processors and 32 GB of RAM. The InGaN simulation files for Silvaco[®] Atlas[®] are included in the SLALOM distribution.

The optimal set of parameters gives an optimal efficiency of about 18 %, a shortcircuit current of 26.8 mA/cm², an open-circuit voltage of 0.85 V and a fill factor of 78 %, obtained for the following set of values: a P-layer thickness of 0.01 μm, an N-layer thickness of 1 μ m, a P-layer doping of 10¹⁹ cm⁻³, an N-layer doping of 4×10¹⁶ cm⁻³ and an Indium composition of 56 %.

OPTIMIZATION OF CZTS BASED SOLAR CELLS

Copper Zinc Tin Selenide Cu₂ZnSnSe₄ (CZTS): abundance of elements and high photovoltaic performances. The CZTS simulation files for Silvaco© Atlas[®] are included in the SLALOM distribution.

The set of parameters choosen to be optimized are the CZTS absorber doping and thickness. The other data used in the simulation, such as the CZTS bandgap, mobilities and absorption coefficient and the CdS layer parameters, are fixed to their experimentally known values.

Optimal efficiency found by SLALOM: 20.5 % for a CZTS thickness of 1.3 μ m and a doping concentration of 1.4×10^{15} cm⁻³. Efficiency is higher than the InGaN solar cell efficiency, showing the potential of this alternative material for photovoltaics.

The optimization duration was about three hours, more than ten times faster than rough parametric analysis.





parameters, ...: taken from literature and/or extracted from experimental data.

Parameters [1]	InN	GaN	CZTS
Bandgap (eV)	0.7	3.42	1.5
Affinity (eV)	5.6	4.1	4.5
Carrier lifetime (ns)	1	1	1000
Permittivity	15.3	8.9	10
N _c (cm ⁻³)	9.1×10 ¹⁷	2.3×10 ¹⁸	2.2×10 ¹⁸
N _v (cm ⁻³)	5.3×10 ¹⁹	4.6×10 ¹⁷	1.8×10 ¹⁹
Absorption	Extracted from experimental data [3]		
Mobility	Caughey-Thomas Model [4]		
Refractive Index	Adachi Model [5]		

[1] E Matioli, C Neufeld, M Iza, S C Cruz, AA AlHeji, X Chen, RM Farrell, S Keller, S DenBaars, and U Mishra. High internal and external quantum efficiency InGaN/GaN solar cells. Applied Physics Letters, 98(2):021102, 2011.

[2] M Jiang and X Yan. Cu 2 ZnSnS 4 thin film solar cells: present status and future prospects. In Solar Cells-Research and Application Perspectives. InTech, 2013.

[3] G Brown, J Ager III, W Walukiewicz and J. Wu, Finite element simulations of compositionally graded InGaN solar cells, Solar Energy Materials and Solar Cells 94 (3) (2010) 478–483.

[4] F Schwierz, An electron mobility model for wurtzite GaN, Solid State Electronics 49 (6) (2005) 889–895.

[5] AB Djurisic, EH Li, Modeling the optical constants of hexagonal GaN, InN, and AlN, Journal of Applied Physics 85 (5) (1999) 2848–2853.

Current-voltage characteristic of the InGaN PN solar cell at the optimum:



[6] S Ould Saad Hamady, A Adaine, and N Fressengeas. Numerical simulation of InGaN Schottky solar cell. Materials Science in Semiconductor Processing, 41:219–225, 2016. [7] A Adaine, S Ould Saad Hamady, and N Fressengeas. Simulation study of a new InGaN p-layer free Schottky based solar cell. Superlattices and Microstructures, 96:121–133, 2016. [8] Abdoulwahab Adaine, Sidi Ould Saad Hamady, and Nicolas Fressengeas. Effects of structural defects and polarization charges in InGaN-based double-junction solar cell. Superlattices and Microstructures, 107:267–277, 2017.