

Comparative study of of PN, PIN and new Schottky based InGaN thin films solar cells

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What is this all about ?

- 1 InGaN Schottky Solar Cell modeling & optimization
 - Modeling the Solar Cell
 - Multi-variate optimization
 - An optimal design
- 2 Proposal for a new InGaN MIN structure
 - Optimal PN and PIN structure
 - Schottky Based InGaN Solar Cells
 - MIN structure behavior
- 3 From simulation to realization
 - InGaN composition
 - Crystal defects
 - Metal work function
 - Future work

InGaN for solar cells

Decisive advantages vs. Technological issues

Continuous solar spectrum covering

- Indium composition change
- Multi-junction solar cells

Robust material

- High temperatures
- Radiation resistant

High light absorption

- Thin layers
- Nanoscale

Lack of lattice matched substrate

- Difficult elaboration
- High defect density

Rough road to the device

- P doping uneasy
 - lack of acceptors
 - natural N doping
- Contact deposition difficult

Optimizing the Schottky design

Removing the need for a p-layer

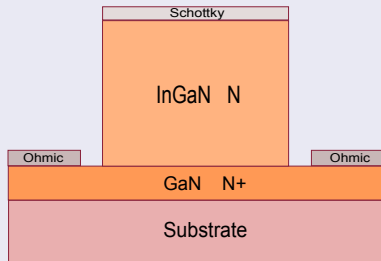
One junction only in this talk

- Get the best out of 1 junction
- First step towards multi-junction

This talk objective

- p-layer free device
- Predict InGaN solar cell efficiency
- Predict the parameter set for the best efficiency
 - Dopings
 - Thicknesses
 - Metal work function

The Schottky design



Modeling and simulation

Experimental data linked to SILVACO™ ATLAS™ 2D state of the art simulator

Simulation framework

- ATLAS™ back-end from SILVACO™
- 2D drift-diffusion non linear differential problem
- Coupled & decoupled methods

InGaN parameters from experiment

- From GaN & InN binaries
- Linear Vegard interpolation for InGaN
- Bowing for affinity & bandgap: 0.8eV & 1.43eV

Carrier Transport

- Caughey-Thomas for mobility
- Recombinations : direct, Auger, SRH and bandgap narrowing
- 1ns carrier lifetime

Solar Light & Absorption

- Standard AM1.5 Solar Spectrum
- Adachi model
- Parameters from polynomial fit

Simulation process

Simulation up and running : inputs and outputs

Input data: photovoltaic cell physical parameters

- N InGaN composition, doping and thickness
- Metal work function
- In short: 4 parameters

Simulation output data: comprehensive electrical analysis

- I-V curves
- Electric field mapping
- ...
- Cell efficiency
- Open circuit Voltage
- Short circuit Current
- I-V Fill Factor

η

V_{oc}

J_{sc}

FF

The need for math

When hand driven parameter variation fails

A multivariate optimization problem

- Efficiency is a function of 4 parameters
- Varying one parameter at a time **fails**

$$\eta : (\mathbb{R}^+)^4 \mapsto \mathbb{R}^+$$

Various multivariate optimization methods

- Brute Force
- Gradient descent
- Conjugate gradient
- ...

Multivariate optimization method

SAGE/python interface to SciPy algorithms

- Formalize ATLAS™ calculations as a multivariate function
- Use the appropriate optimization method on it

Choosing the optimization method

- Gradient and Hessian have to be approximated
- Problem bounded by physics and technology
- Bounded approximate gradient methods

The question of the starting point

- Several random starting points
- To ensure maximum efficiency uniqueness

InGaN Schottky Solar Cell optimal design¹

Using very loose technological constraints

Optimal 18.2% efficiency with 10% tolerance

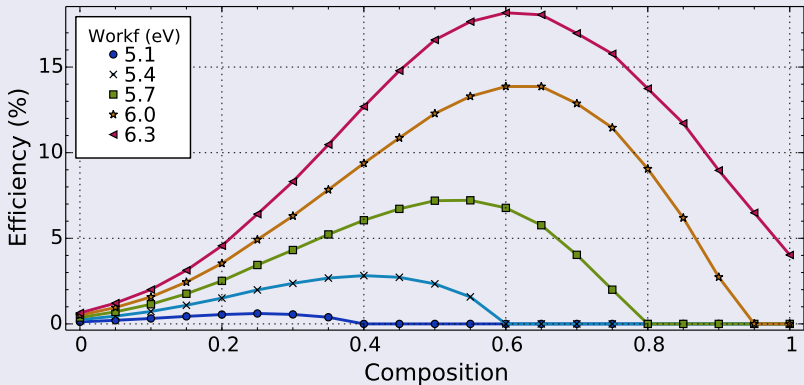
	$L_n(\mu m)$	$N_d(cm^{-3})$	$W_f(eV)$	x	$\eta(\%)$ $V_{OC}(V)$ $J_{SC}(mA/cm^2)$ $FF(\%)$
Range	[0.10 – 1.00]	$[1.0 \times 10^{16} - 1.0 \times 10^{19}]$	[5.50 – 6.30]	[0.00 – 1.00]	
Schottky	0.86 [0.53 – 1.00]	6.5×10^{16} [$1.0 \times 10^{16} - 3.0 \times 10^{17}$]	6.30 [6.15 – 6.30]	0.56 [0.50 – 0.72]	18.2 0.863 26.80 78.82

¹ *Materials Science in Semiconductor Processing*, 2016, 41, pp.219-225.

Varying metal work function and composition

around the optimal values

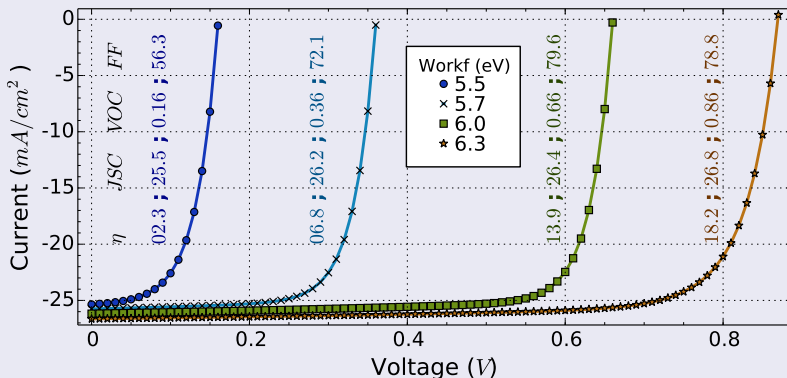
Changing work function and composition modulates SCR



I - V for various work functions

around the optimal values

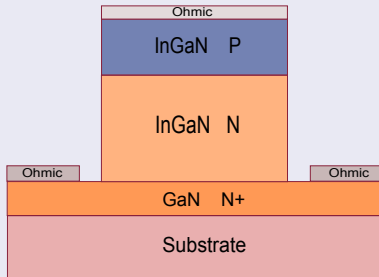
The efficiency increase is mainly due to V_{OC} increase



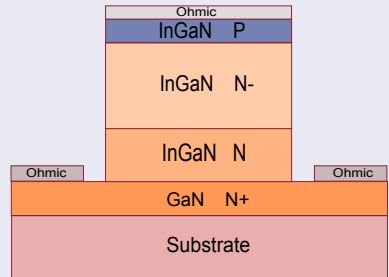
InGaN PN & PIN structure optimal designs

PN & PIN are standard structures worth optimizing

PN InGaN PV Cell



PIN InGaN PV Cell



InGaN is naturally n-doped

InGaN I layer is actually slightly N doped

Optimal InGaN PN & PIN : 17.8% & 19% efficiency

Notice the huge 90% tolerances and the ultra-small P layer

	$L_p(\mu m)$	$L_n(\mu m)$	$N_a(cm^{-3})$	$N_d(cm^{-3})$	x	$\eta(\%)$ $V_{OC}(V)$ $J_{SC}(mA/cm^2)$ $FF(\%)$
Range	[0.01 – 1.00]	[0.10 – 1.00]	$[10^{16} - 10^{19}]$	$[10^{16} - 10^{19}]$	[0.00 – 1.00]	
PN	0.01 [0.01 – 0.04]	1.00 [0.48 – 1.00]	10^{19} [$4.4 \times 10^{16} - 10^{19}$]	3.9×10^{16} [$10^{16} - 3.5 \times 10^{17}$]	0.56 [0.50 – 0.72]	17.8 0.855 26.75 77.85
PIN	0.01 [0.01 – 0.04]	0.50 [0.10 – 1.00]	10^{19} [$5.9 \times 10^{16} - 10^{19}$]	5.0×10^{17} [$1.9 \times 10^{16} - 10^{19}$]	0.59 [0.47 – 0.71]	19.0 0.875 27.36 79.39

- I layer optimal thickness : $0.54\mu m$
- I layer thickness 90% tolerance : $[0.18 - 1]\mu m$
- I layer optimal n-doping : $5.8 \times 10^{16}cm^{-3}$
- I layer n-doping 90% tolerance : $[10^{14} - 10^{17}]cm^{-3}$

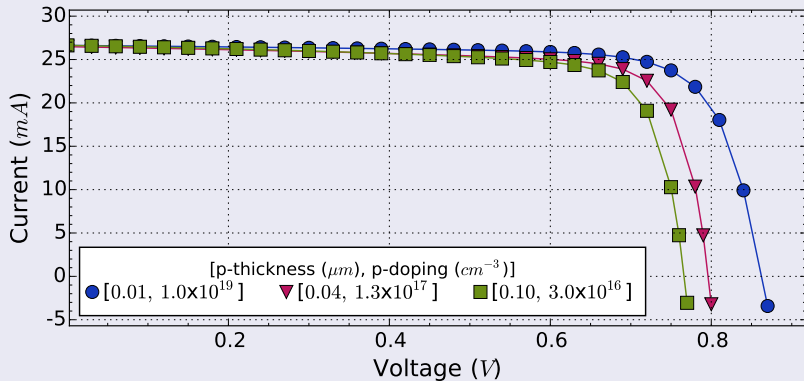
Nanoscale P layer : suggests P layer removal

Optimal InGaN PN Current-Voltage characteristics

Fixing the p-thickness and finding the optimal p-doping associated to it

For several optimal (p-thickness, p-doping) couples

PN

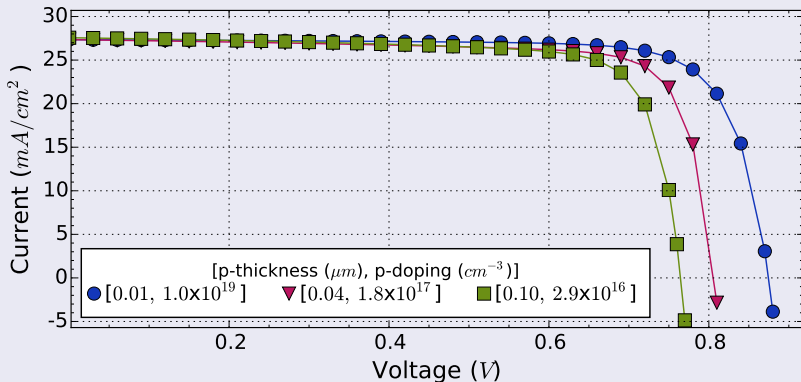


Optimal InGaN PIN Current-Voltage characteristics

Fixing the p-thickness and finding the optimal p-doping associated to it

For several optimal (p-thickness, p-doping) couples

PIN

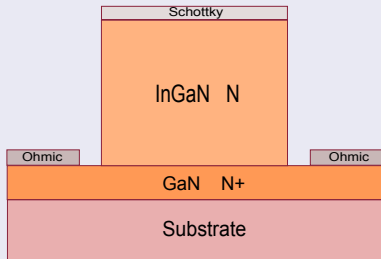


Schottky Based InGaN Solar Cell

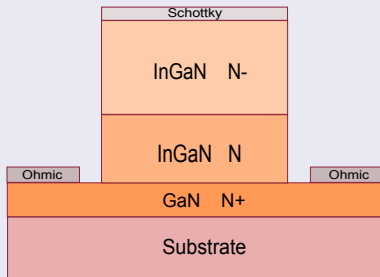
(SBSC)

P layer removed and replaced by a Schottky contact

Schottky InGaN PV Cell



New Metal-IN InGaN PV Cell



InGaN is naturally n-doped

InGaN I layer is actually slightly N doped

Optimal InGaN Schottky & Metal-IN Solar Cells

Huge tolerances

Up to 18.2% & 19.8% efficiency

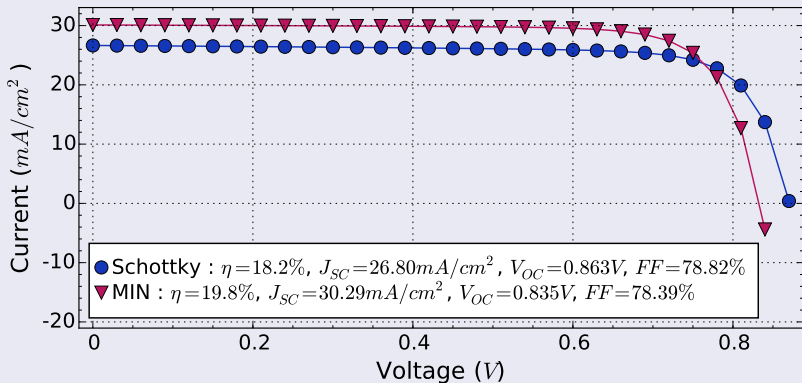
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Schottky	0.86 [0.53 – 1.00]	6.5×10^{16} [1.0×10^{16} – 3.0×10^{17}]	6.30 [6.15 – 6.30]	0.56 [0.50 – 0.72]	18.2 0.863 26.80 78.82
MIN	0.83 [0.10 – 1.00]	3.6×10^{17} [1.8×10^{16} – 1.0×10^{19}]	6.30 [6.11 – 6.30]	0.60 [0.48 – 0.72]	19.8 0.835 30.29 78.39

- I layer optimal thickness : $0.61\mu m$
- I layer thickness 90% tolerance : $[0.1 - 1]\mu m$
- I layer optimal n-doping : $6.1 \times 10^{16}cm^{-3}$
- I layer n-doping 90% tolerance : $[10^{14} - 10^{17}]cm^{-3}$

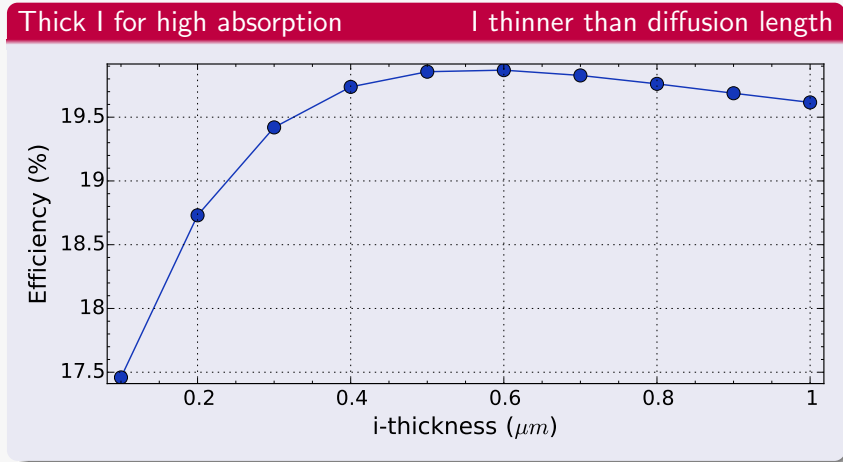
InGaN Schottky and MIN Current-Voltage characteristics

V_{OC} : Indium composition

J_{SC} : Solar light absorption



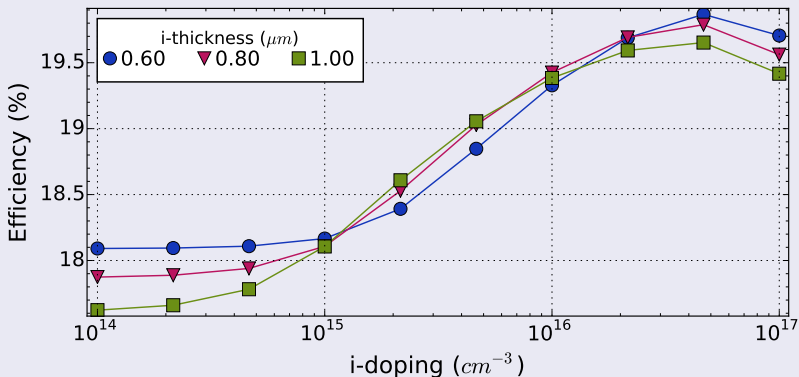
MIN PV efficiency as a function of the i-layer thickness



MIN PV efficiency as a function of i-doping

for various i-thicknesses

Optimal I-doping for optimal Space Charge Region



Optimal InGaN 0.60 composition is still difficult to achieve

Even more if several hundreds of nanometers are required

Recent (2015) experimental work reports 0.22 composition

- Limit In composition to 0.22
- Limit thickness to 400nm

Huge tolerances

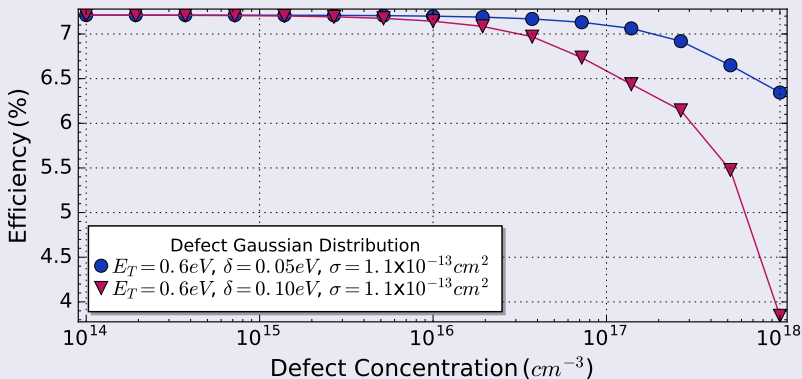
7.25% efficiency

	$L_i(\mu m)$	$L_n(\mu m)$	$N_i(cm^{-3})$	$N_d(cm^{-3})$	$W_r(eV)$	x	$\eta(\%)$ $V_{OC}(V)$ $J_{SC}(mA/cm^2)$ $FF(\%)$
Range	[0.10 – 0.40]	[0.10 – 0.40]	$[1.0 \times 10^{14} - 1.0 \times 10^{17}]$	$[1.0 \times 10^{16} - 1.0 \times 10^{19}]$	[5.50 – 6.30]	[0 – 0.22]	
MIN	0.40 [0.18 – 0.40]	0.40 [0.29 – 0.40]	6.27×10^{15} $[4.6 \times 10^{14} - 2.2 \times 10^{16}]$	7.46×10^{16} $[2.0 \times 10^{16} - 1.0 \times 10^{18}]$	6.30 [6.20 – 6.30]	0.22 [0.19 – 0.22]	7.25 1.438 5.92 85.2

Efficiency degraded by crystalline defects

Urbach tails & Gaussian distribution of defects in the band gap

Defect density must be kept lower than i-layer doping



Efficiency lowering with metal work function lowering

Possible defects not included

Both optimal and experimental compositions

Zero defect efficiency with varying work function

W_f (eV)	η for $x = 0.60$ (%)	η for $x = 0.22$ (%)
6.30	19.80	7.25
6.10	17.84	6.15
5.93	13.58	5.22
5.65	6.34	3.70

Today state of the art device realization : 3.70% efficiency

Future work

Connect to experiments

Contact me

- Collaborate with **experimental groups**
- Study their own technological constraints
- Include them in the optimization
- Realize and test the actual device
- Original approach to be adapted to other materials for PV

Details in two recently published paper

(2016)

- Numerical simulation of InGaN Schottky solar cell
- Simulation study of a new InGaN p-layer free Schottky based solar cell
- Available on ArXiv, HAL and in Elsevier journals