

New Optimized InGaN Metal-IN Solar Cell

China France 2nd Workshop on Advanced Materials
Materials for Energy Session

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Wednesday Aug. 31st, 2016

What is this all about ?

- 1 InGaN Solar Cells modeling & optimization
 - Modeling the Solar Cell
 - Multi-variate optimization
 - Optimal Design
- 2 A new MIN Solar Cell
 - Schottky Based InGaN Solar Cells
 - MIN structure behavior
- 3 From simulation to realization
 - InGaN composition
 - Crystal defects
 - Metal work function
 - Future work

And now...

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InGaN for solar cells

Decisive advantages vs. Technological issues

Continuous solar spectrum covering

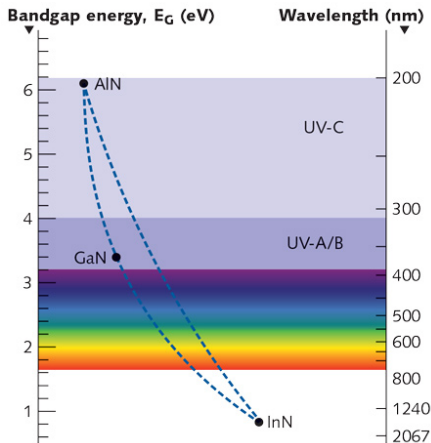
- Indium composition change
- Multi-junction solar cells

Robust material

- High temperatures
- Radiation resistant

High light absorption

- Thin layers
- Nanoscale



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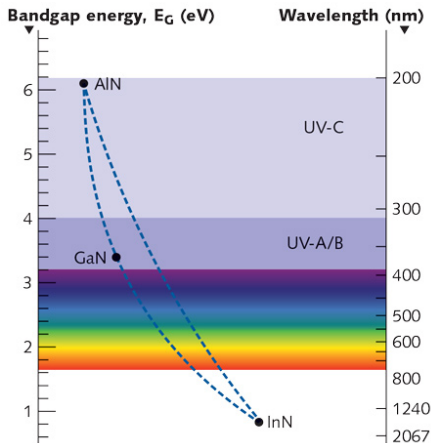
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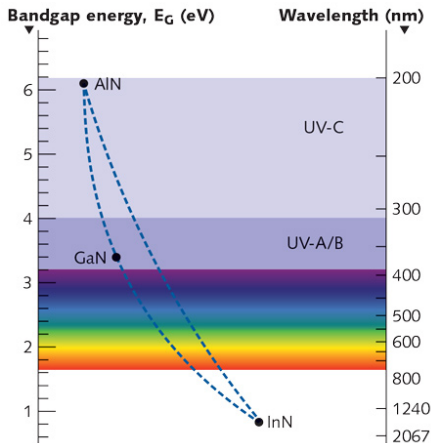
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Lack of lattice matched substrate

- Difficult elaboration
- High defect density

Rough road to the device

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

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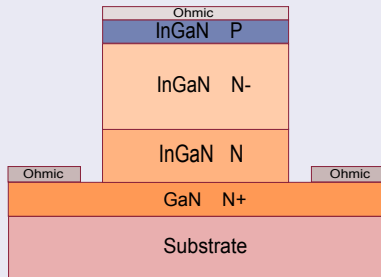
Optimizing the PIN design²

... as an example

One junction only in this talk

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

The PIN design



² *Superlattices and Microstructures*, Elsevier, 2016, 96, pp.121-133.

Optimizing the PIN design²

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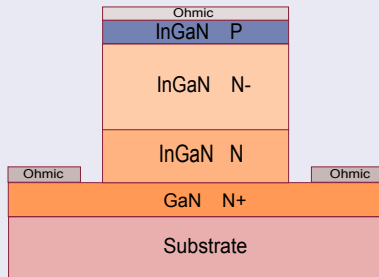
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This talk objective

- Predict InGaN solar cell efficiency
- Predict the parameter set for the best efficiency

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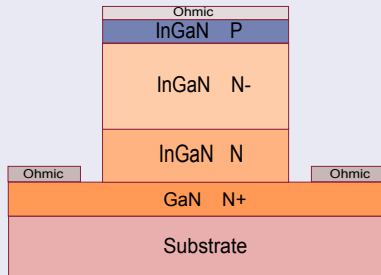
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Modeling and simulation

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
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Simulation process

Simulation up and running : inputs and outputs

Input data: photovoltaic cell physical parameters

- P, I and N InGaN compositions, dopings and thicknesses
- In short: 9 parameters

Simulation output data: comprehensive electrical analysis

- I-V curves
- Electric field mapping
- ...

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V_{oc}

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The need for math

When hand driven parameter variation fails

A multivariate optimization problem

- Efficiency is a function of 9 parameters
- Varying one parameter at a time **fails**

$$\eta : (\mathbb{R}^+)^9 \mapsto \mathbb{R}^+$$

Various multivariate optimization methods

- Brute Force (not usable in 9 dimensions)
- Gradient descent
- Conjugate gradient
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Multivariate optimization method

SAGE/python interface to SciPy algorithms

- Formalize ATLASTM 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

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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 : $[10^{14} - 10^{17}]cm^{-3}$

Huge tolerances : **robust device**

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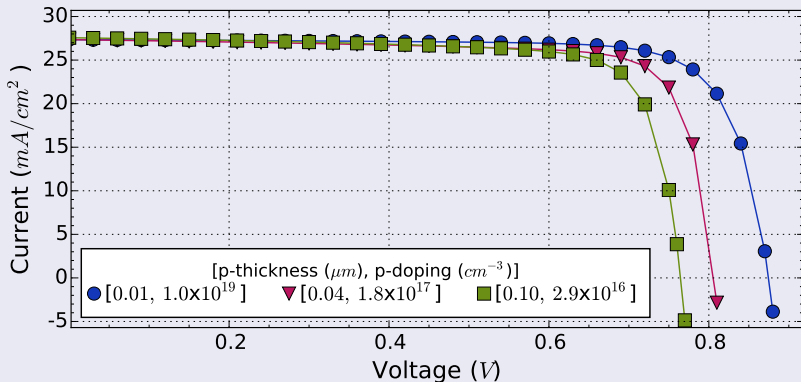
Nanoscale P layer : suggests P layer removal

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



And now...

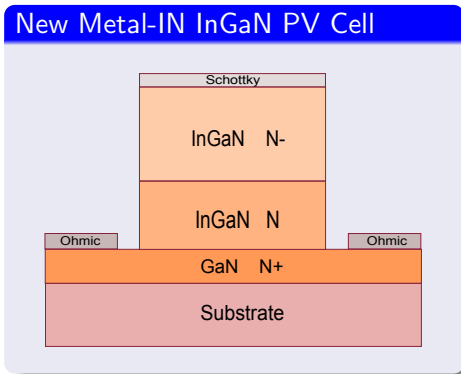
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Schottky Based InGaN Solar Cell²

P layer removed and replaced by a Schottky contact

(SBSC)

Workfunction : W_f



InGaN is naturally n-doped

InGaN I layer is actually slightly N doped

² *Superlattices and Microstructures*, Elsevier, 2016, 96, pp.121-133.

Optimal InGaN Schottky & Metal-IN Solar Cells

Huge tolerances

Up to 18.2% & 19.8% efficiency

	$L_n(\mu m)$	$N_d(cm^{-3})$	$W_f(eV)$	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
MIN	0.83 [0.10 – 1.00]	3.6×10^{17} [$1.8 \times 10^{16} - 1.0 \times 10^{19}$]	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 : $[10^{14} - 10^{17}]cm^{-3}$

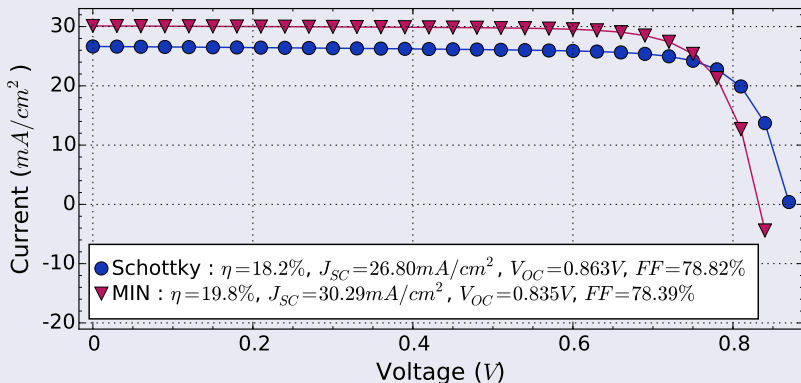
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InGaN Schottky and MIN Current-Voltage characteristics

V_{OC} : Indium composition

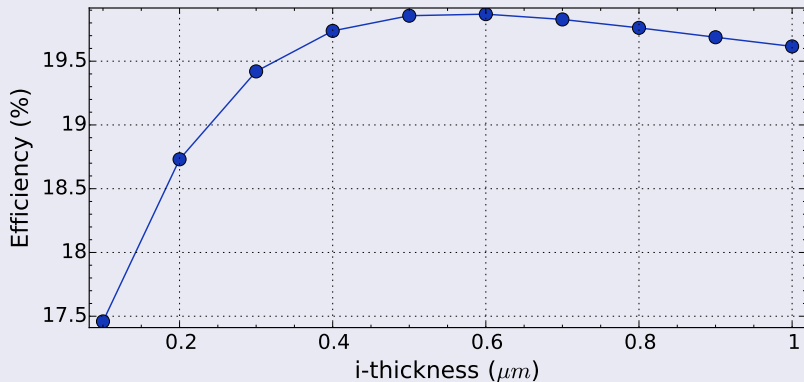
J_{SC} : Solar light absorption



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

Thick I for high absorption

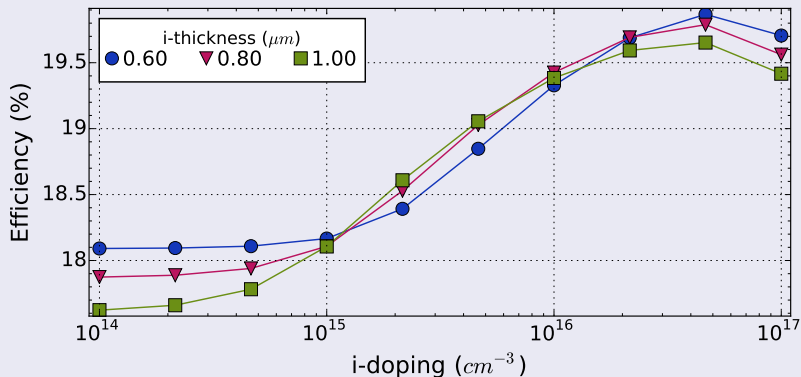
I thinner than diffusion length



MIN PV efficiency as a function of i-doping

for various i-thicknesses

Optimal I-doping for optimal Space Charge Region



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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

	$L_i(\mu m)$	$L_n(\mu m)$	$N_i(cm^{-3})$	$N_d(cm^{-3})$	$W_i(eV)$	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	0.40	6.27×10^{15}	7.46×10^{16}	6.30	0.22	7.25 1.438
	[0.18 – 0.40]	[0.29 – 0.40]	$[4.6 \times 10^{14} - 2.2 \times 10^{16}]$	$[2.0 \times 10^{16} - 1.0 \times 10^{18}]$	[6.20 – 6.30]	[0.19 – 0.22]	5.92 85.2

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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]	
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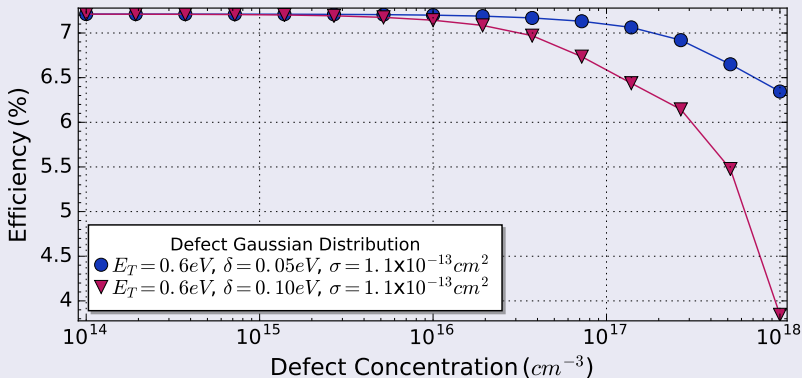
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Efficiency degraded by crystalline defects

Urbach tails & Gaussian distribution of defects in the band gap

Defect density must be kept lower than i-layer doping



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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

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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)

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