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Multivariate numerical optimization of an InGaN-based hetero junction solar cell



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Summary

Because of remarkable properties of InGaN, we simulated and optimized an InGaN-based dual-junction solar cell connected by a specifically designed tunnel junction. The device is simulated in the framework of a drift-diffusion model using the ATLAS device simulation framework from the Silvaco company. The optimization is done by coupling ATLAS with multivariate mathematical optimization methods based on state-of-the-art optimization algorithms. For that, we used a Python package that we developed in the SAGE software interface. The objective is to optimize the conversion efficiency of the solar cell by simultaneously optimizing several physical and geometrical parameters of the solar cell. It is an unprecedented multivariate optimization for solar cells which takes into account the correlation between these parameters. For this solar cell, we optimized simultaneously 11 parameters of the structure. An optimum conversion efficiency of 24% was predicted for this designed solar cell.

Multivariate Optimization

Standard-Method: Parametric Analysis

- One parameter is varying while the other parameters are kept **constant**
- Have not taken into account, the complexity of the **interdependence** of parameters
- Application difficult to design components

Our Method: Multivariate Optimization

- Simultaneously** optimizing of several **physical** and **geometrical** parameters
- Much more **rigorous** than **single parametric analysis**
- Suitable for next generation solar cell
- Optimum efficiency** as a function of several optimization parameters

Mathematical Optimization

- Three algorithms (state-of-the-art)**
- 1- **TNC** (Truncated Newton Algorithm)
- 2- **SLSQP** (Sequential Least Squares Programming)
- 3- **L-BFGS-B** (Quasi-Newton Method)

Sage/Scipy

- We use the Sage software interface to the Scipy optimizers
- Open source free software
- Coded and optimized by computer experts

Numerical Simulation

Multivariate Optimization

Simulation: Drift-Diffusion Model

Current equations

$$J_n = qn\mu_n E + qD_n \frac{dn}{dx}$$
$$J_p = qp\mu_p E + qD_p \frac{dp}{dx}$$

Poisson's equation

$$\nabla E = \frac{\rho}{\epsilon_0}$$

- q : electronic charge, n : electron density,
- p : electron density, μ : carrier mobility,
- E : Electric field, D : Diffusion coefficient.
- ρ : Charge density ϵ_0 : Permittivity

Using ATLAS

(Silvaco company software)

Physical modeling using Experimental data to tune well known models:

- Carrier Mobility** :
Caughey-Thomas model
- Carrier Recombination** :
Shockley-Read-Hall (SRH) , direct and Auger recombination models
- Index of refraction** :
Adachi model
- Absorption coefficient** :
Phenomenological Model

Multijunction InGaN Solar Cell

Solar Cell Structure

InGaN-based double-junction solar cell

- Structure composed of **two p-n junctions**
- Two subcell vertically stacked having different **bandgaps**

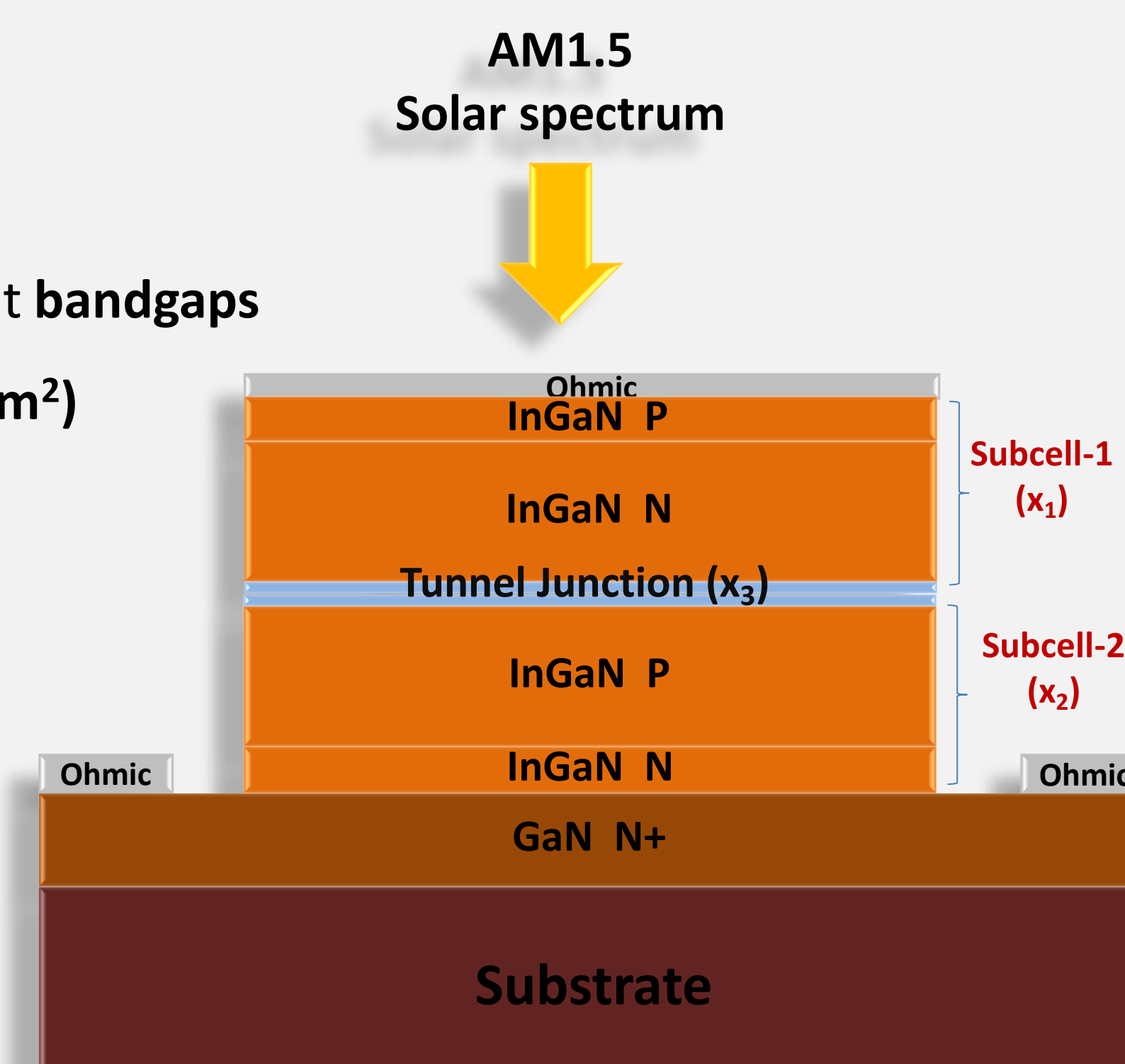
Structure under AM1.5 illumination (100mW/cm²)

- Subcell-1, absorbs **high-energy** photons
- Subcell-2, absorbs **lower energies** photons
- The Solar cell absorbs a larger solar spectrum than a single junction cell

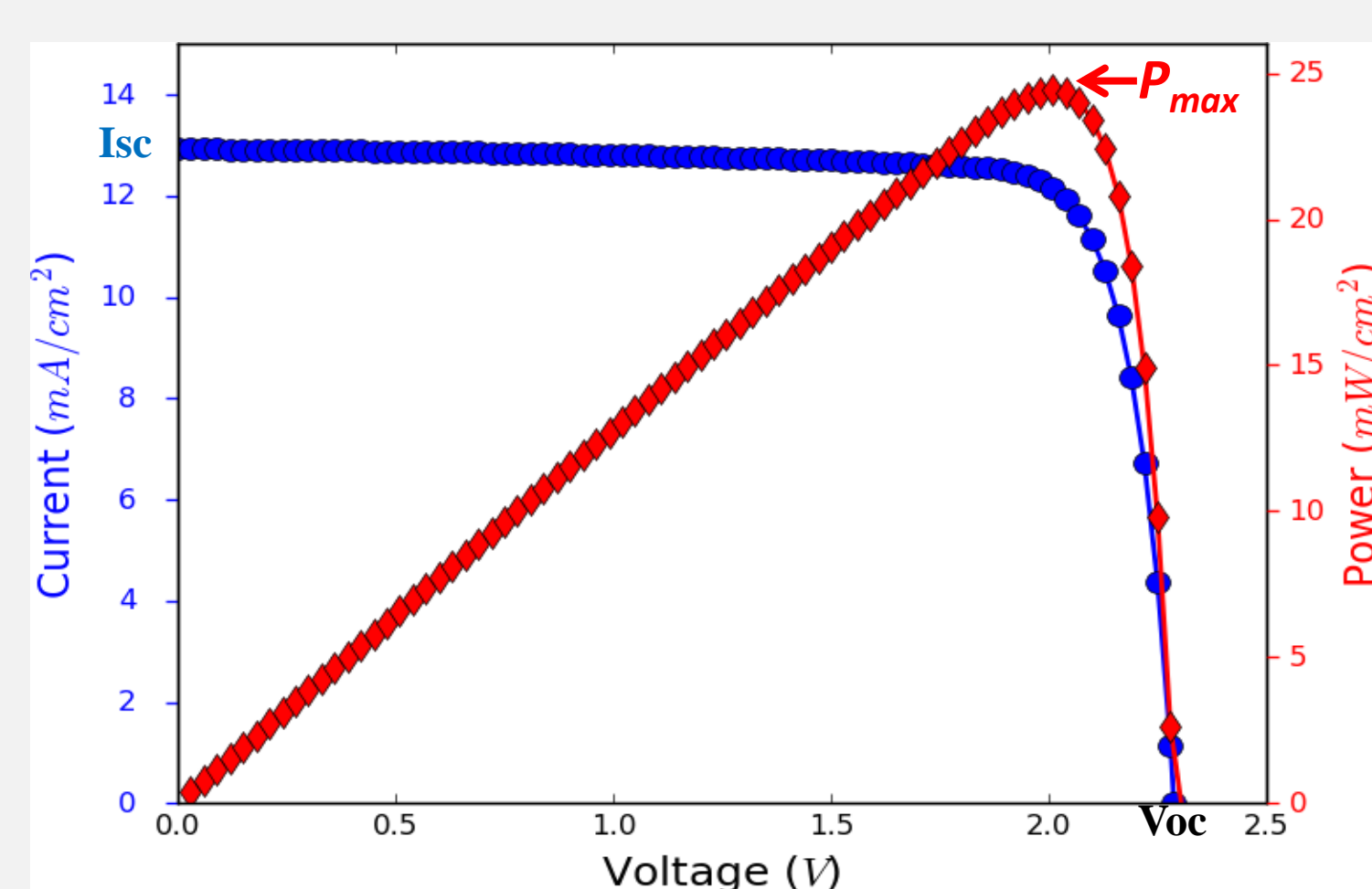
Tunnel junction

- The two subcells are connected by a tunnel junction to enhance current matching between the subcells

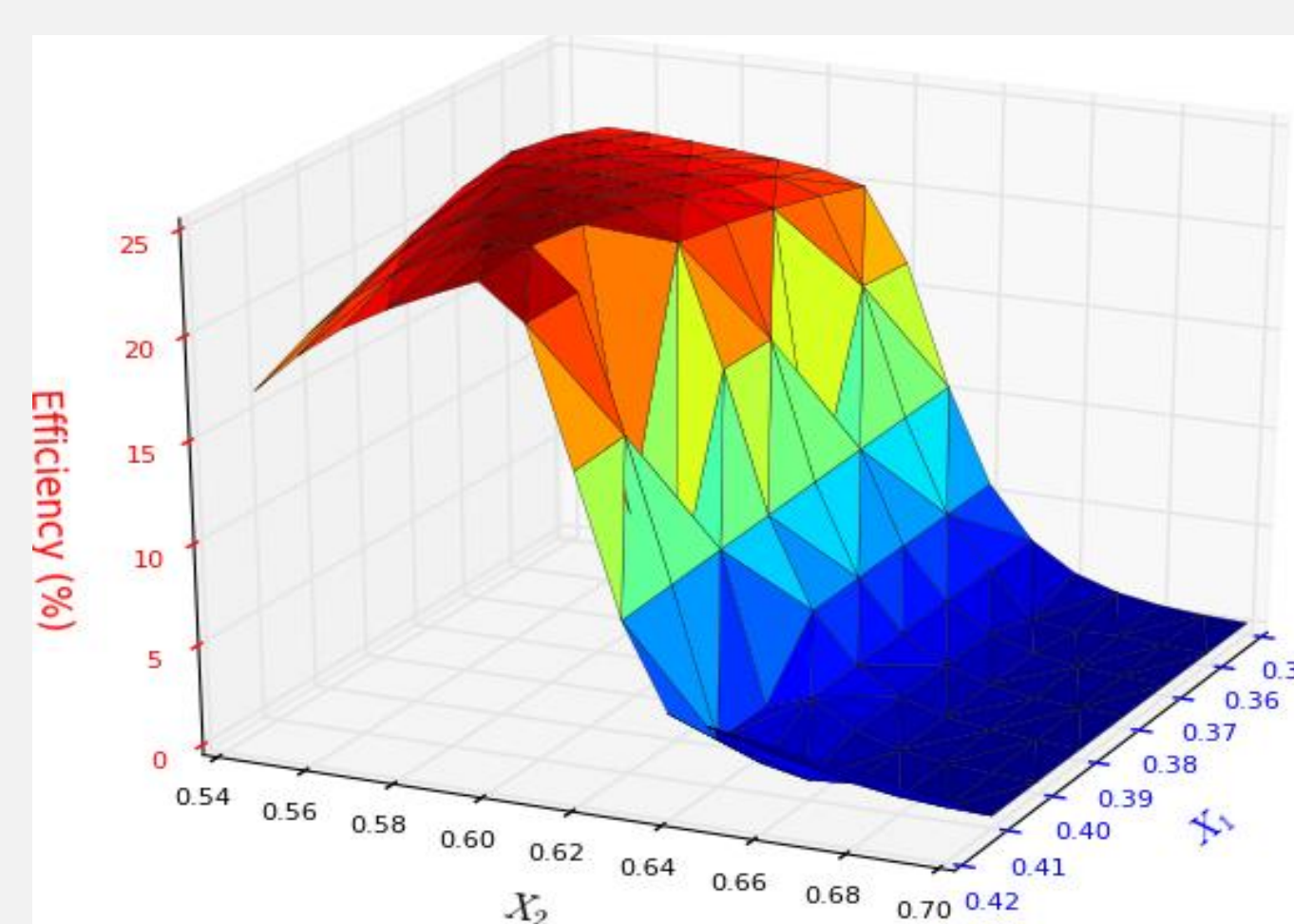
- x_1 , x_2 and x_3 Indium composition of subcell-1, subcell-2 and tunnel junction respectively



Solar Cell Performances



Current-voltage and power-voltage characteristic curves. P_{max} the maximum power of solar cell



Efficiency as a function of the Indium compositions, x_1 for the top cell and x_2 for the bottom cell

Optimal Results

11 Parameters of solar cell are optimized simultaneously

- Obviously the optimization problem becomes more complex with so many variables
- Optimization method with a higher-order convergence
- Ensure the overall convergence of the optimization method

11 Optimization parameters concerns the **dopings** and the **thicknesses** of the **2 subcells** and the different **indium compositions** (x_1 , x_2 , x_3).

Their optimization intervals are as follows:

- The Indium composition is x in $In_xGa_{(1-x)}N$: $[0.00 - 1.00]$
- The InGaN layer n-type and p-type doping : $[1.10^{16} - 1.10^{19}]cm^{-3}$
- The InGaN layer thickness : $[0.01 - 1.00]\mu m$

Their optimal values are in the following table:

Subcell-1	P-Layer	1) Thickness (nm)	0.01	9) $x_1 = 0.40$
	N-Layer	2) Doping (cm ⁻³)	8.04×10^{18}	
Tunnel Junction		3) Thickness (nm)	0.58	10) $x_3 = 0.50$
		4) Doping (cm ⁻³)	2.38×10^{16}	
Subcell-2	P-Layer	5) Thickness (nm)	0.57	11) $x_2 = 0.59$
	N-Layer	6) Doping (cm ⁻³)	2.51×10^{18}	
		7) Thickness (nm)	0.01	
		8) Doping (cm ⁻³)	1.00×10^{17}	

Optimal efficiency and the significant parameters of the solar cell

$\eta=24.4\%$

The short-circuit current, $J_{sc} = 12.92mA/cm^2$

The open-circuit voltage, $V_{oc} = 2.287V$

Fill factor,

$FF = 82.55$