

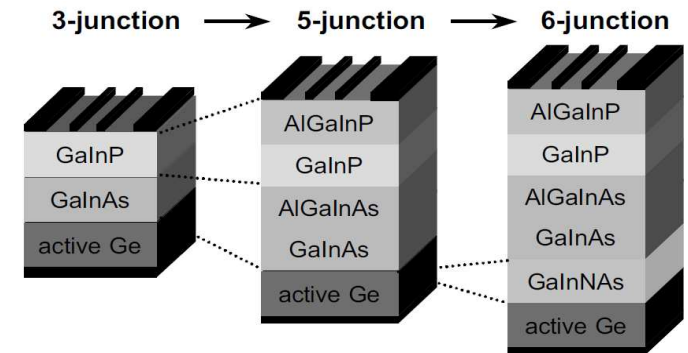


# **PVcell** – software for modeling semiconductor solar cells



# General description of the simulator

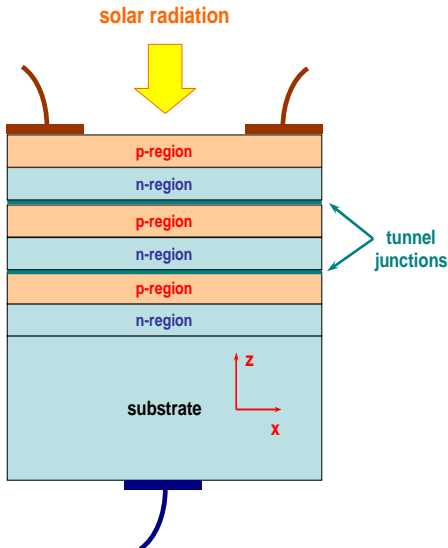
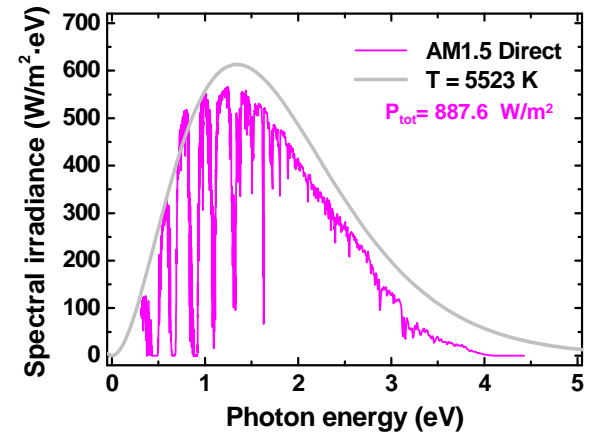
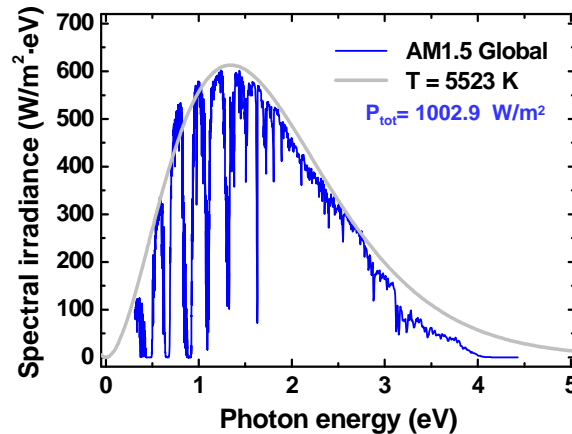
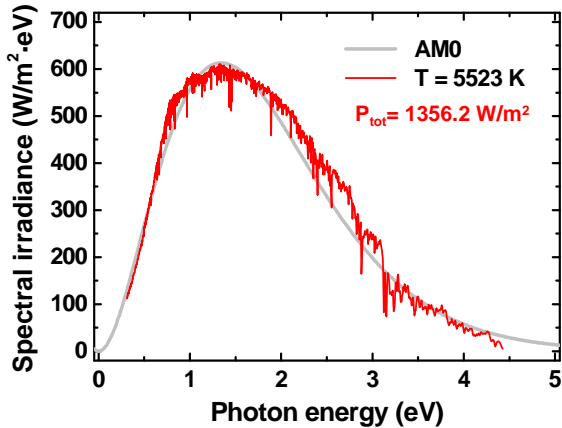
- ✓ Simple p-n junction and tandem solar cells made of various inorganic semiconductor materials
- ✓ Materials systems: Si, Ge, conventional III-V binary compounds and alloys, III-nitride and II-oxide wurtzite semiconductors and alloys
- ✓ Bulk semiconductor layers, multiple-quantum wells, and superlattices with possible account of partial strain relaxation
- ✓ Quasi-1D approach providing fast and efficient simulations



Physics Laboratory physics.nist.gov					Standard Reference Data Group www.nist.gov/srd																																												
13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18	19	20	21	22																																								
5 <sup>3</sup> P <sub>1/2</sub> B Boron 10.811 1s <sup>2</sup> 2s <sup>2</sup> 2p	6 <sup>3</sup> P <sub>0</sub> C Carbon 12.0107 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>2</sup>	7 <sup>3</sup> P <sub>1/2</sub> N Nitrogen 14.0067 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>3</sup>	8 <sup>3</sup> P <sub>0</sub> O Oxygen 15.9994 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>4</sup>	9 <sup>3</sup> P <sub>3/2</sub> F Fluorine 18.99840322 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>5</sup>	10 <sup>3</sup> P <sub>3/2</sub> Ne Neon 20.1797 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup>	11 <sup>3</sup> P <sub>3/2</sub> Na Sodium 22.98976928 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup> 3s <sup>1</sup>	12 IIB Zn Zinc 65.409 [Ar]3d <sup>10</sup> 4s <sup>1</sup> 9.3942	13 <sup>3</sup> P <sub>1/2</sub> Al Aluminum 26.981538 [Ne]3s <sup>2</sup> 3p 5.9858	14 <sup>3</sup> P <sub>0</sub> Si Silicon 28.0855 [Ne]3s <sup>2</sup> 3p 8.1517	15 <sup>3</sup> S <sub>1/2</sub> P Phosphorus 30.973761 [Ne]3s <sup>2</sup> 3p 10.4867	16 <sup>3</sup> P <sub>0</sub> S Sulfur 32.065 [Ne]3s <sup>2</sup> 3p 10.3600	17 <sup>3</sup> P <sub>3/2</sub> Cl Chlorine 35.453 [Ne]3s <sup>2</sup> 3p 12.370	18 <sup>3</sup> P <sub>3/2</sub> Ar Argon 39.948 [Ne]3s <sup>2</sup> 3p 15.7596	19 <sup>3</sup> P <sub>3/2</sub> K Potassium 39.0983 [Ar]4s <sup>1</sup>	20 <sup>3</sup> P <sub>3/2</sub> Ca Calcium 40.078 [Ar]4s <sup>2</sup>	21 <sup>3</sup> P <sub>3/2</sub> Sc Scandium 44.955912 [Ar]3d <sup>1</sup> 4s <sup>2</sup>	22 <sup>3</sup> P <sub>3/2</sub> Ti Titanium 47.88 [Ar]3d <sup>2</sup> 4s <sup>2</sup>	23 <sup>3</sup> P <sub>3/2</sub> V Vanadium 50.9415 [Ar]3d <sup>3</sup> 4s <sup>2</sup>	24 <sup>3</sup> P <sub>3/2</sub> Cr Chromium 51.99616 [Ar]3d <sup>5</sup> 4s <sup>1</sup>	25 <sup>3</sup> P <sub>3/2</sub> Mn Manganese 54.938044 [Ar]3d <sup>5</sup> 4s <sup>2</sup>	26 <sup>3</sup> P <sub>3/2</sub> Fe Iron 55.845 [Ar]3d <sup>6</sup> 4s <sup>2</sup>	27 <sup>3</sup> P <sub>3/2</sub> Co Cobalt 58.933195 [Ar]3d <sup>7</sup> 4s <sup>2</sup>	28 <sup>3</sup> P <sub>3/2</sub> Ni Nickel 58.6934 [Ar]3d <sup>8</sup> 4s <sup>2</sup>	29 <sup>3</sup> P <sub>3/2</sub> Cu Copper 63.546 [Ar]3d <sup>10</sup> 4s <sup>1</sup>	30 <sup>3</sup> P <sub>3/2</sub> Zn Zinc 65.409 [Ar]3d <sup>10</sup> 4s <sup>1</sup> 9.3942	31 <sup>3</sup> P <sub>1/2</sub> Ga Gallium 69.723 [Ar]3d <sup>10</sup> 4s <sup>1</sup> 9.9993	32 <sup>3</sup> P <sub>0</sub> Ge Germanium 72.64 [Ar]3d <sup>10</sup> 4s <sup>1</sup> 7.8904	33 <sup>3</sup> S <sub>1/2</sub> As Arsenic 74.92160 [Ar]3d <sup>10</sup> 4s <sup>1</sup> 9.7886	34 <sup>3</sup> P <sub>0</sub> Se Selenium 78.96 [Ar]3d <sup>10</sup> 4s <sup>1</sup> 9.7524	35 <sup>3</sup> P <sub>3/2</sub> Br Bromine 79.904 [Ar]3d <sup>10</sup> 4s <sup>1</sup> 1.8138	36 <sup>3</sup> P <sub>3/2</sub> Kr Krypton 83.798 [Ar]3d <sup>10</sup> 4s <sup>1</sup> 13.9996	37 <sup>3</sup> P <sub>3/2</sub> Rb Rubidium 85.4678 [Kr]4d <sup>1</sup> 5s <sup>1</sup>	38 <sup>3</sup> P <sub>3/2</sub> Sr Strontium 87.62 [Kr]4d <sup>1</sup> 5s <sup>2</sup>	39 <sup>3</sup> P <sub>3/2</sub> Y Yttrium 88.905848 [Kr]4d <sup>1</sup> 5s <sup>2</sup>	40 <sup>3</sup> P <sub>3/2</sub> Zr Zirconium 91.224 [Kr]4d <sup>2</sup> 5s <sup>2</sup>	41 <sup>3</sup> P <sub>3/2</sub> Nb Niobium 92.90638 [Kr]4d <sup>4</sup> 5s <sup>1</sup>	42 <sup>3</sup> P <sub>3/2</sub> Mo Molybdenum 95.94 [Kr]4d <sup>5</sup> 5s <sup>1</sup>	43 <sup>3</sup> P <sub>3/2</sub> Tc Technetium 98.90625 [Kr]4d <sup>5</sup> 5s <sup>2</sup>	44 <sup>3</sup> P <sub>3/2</sub> Ru Ruthenium 101.07 [Kr]4d <sup>6</sup> 5s <sup>1</sup>	45 <sup>3</sup> P <sub>3/2</sub> Rh Rhodium 102.90550 [Kr]4d <sup>7</sup> 5s <sup>1</sup>	46 <sup>3</sup> P <sub>3/2</sub> Pd Palladium 106.42 [Kr]4d <sup>10</sup>	47 <sup>3</sup> P <sub>3/2</sub> Ag Silver 107.8682 [Kr]4d <sup>10</sup> 5s <sup>1</sup>	48 <sup>3</sup> P <sub>3/2</sub> Cd Cadmium 112.411 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 8.9938	49 <sup>3</sup> P <sub>1/2</sub> In Indium 114.818 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5.7864	50 <sup>3</sup> P <sub>0</sub> Sn Tin 118.710 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 7.3439	51 <sup>3</sup> S <sub>1/2</sub> Sb Antimony 121.760 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 8.0084	52 <sup>3</sup> P <sub>0</sub> Te Tellurium 127.60 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 9.0090	53 <sup>3</sup> P <sub>3/2</sub> I Iodine 126.90447 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 10.4513	54 <sup>3</sup> P <sub>3/2</sub> Xe Xenon 131.293 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 12.1298



- ✓ a number of tabulated solar radiation spectra are available

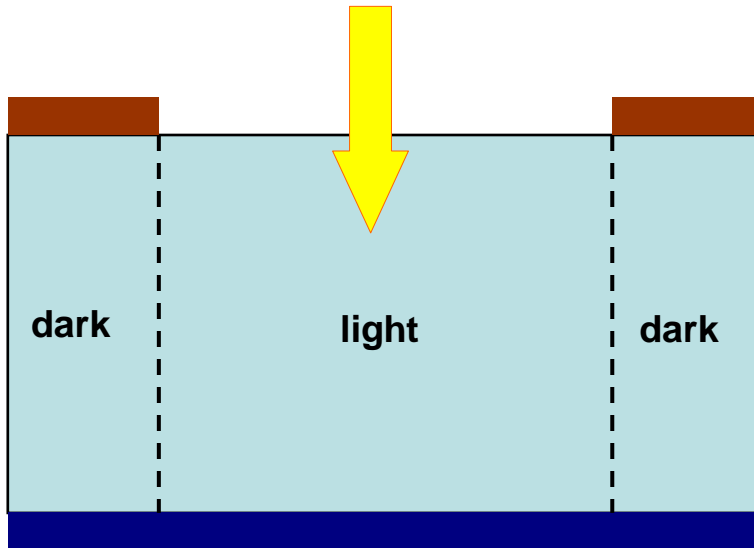


- ✓ concentration factor (in 'suns')
- ✓ optical properties of the top and bottom surfaces, including multi-layer coatings; a way of the SC structure illumination
- ✓ heterostructure design, including combination of different materials systems; degree of strain relaxation in every particular epilayer and some materials properties



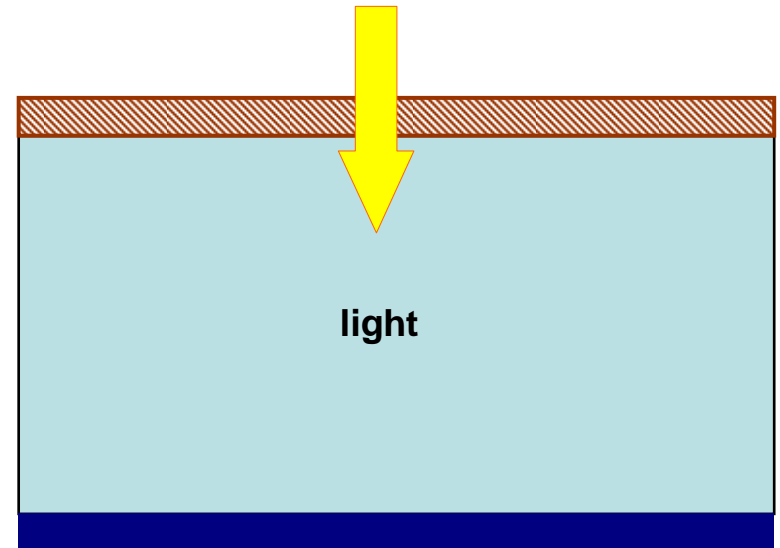
Real device (2D)

solar radiation



Model device (1D)

solar radiation

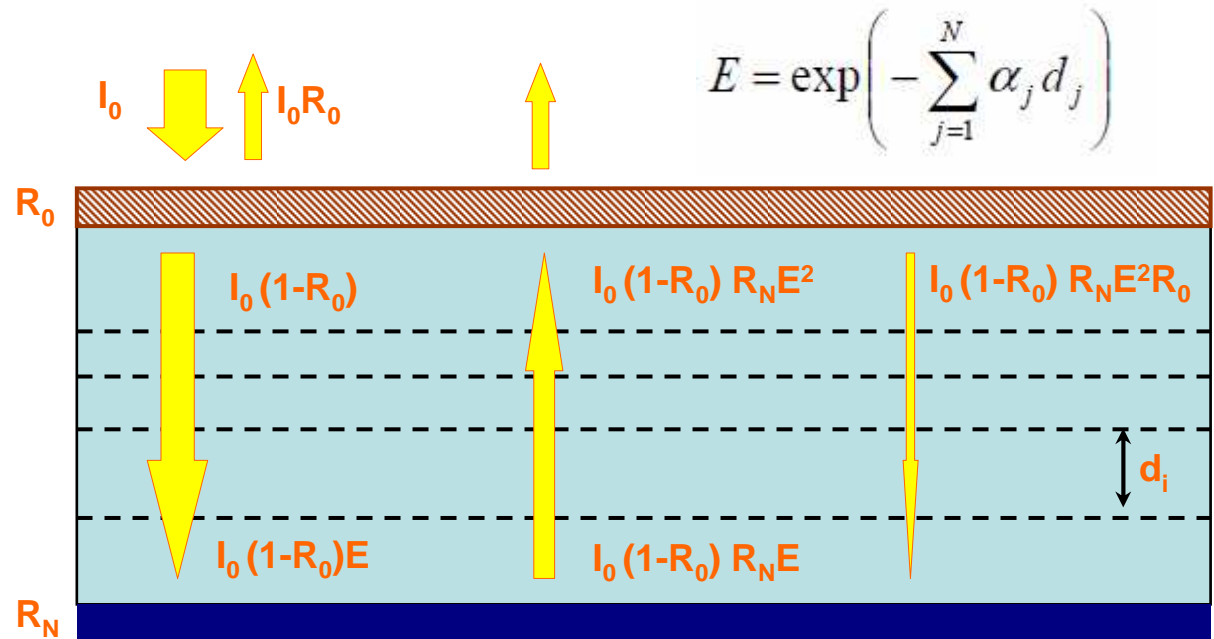


- ✓ Bottom contact is assumed to be a reflective Ohmic contact
- ✓ Top contact is assumed to be a transparent Ohmic contact



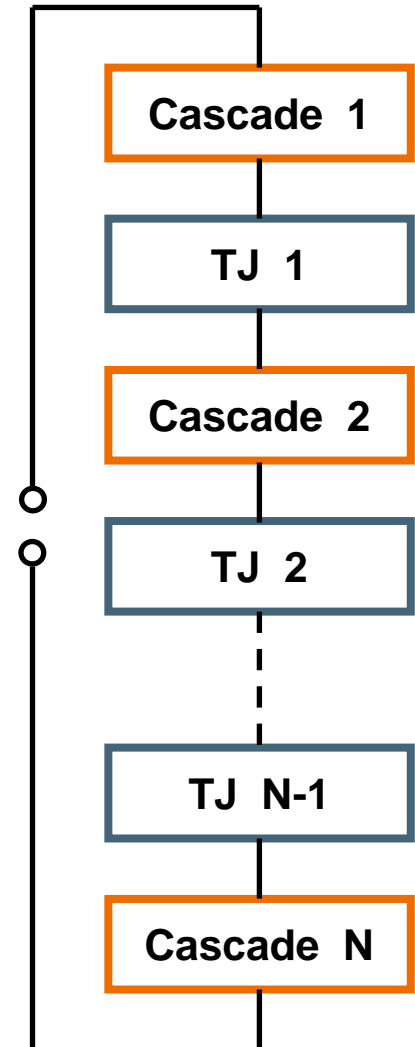
# Light absorption model

For each wavelength, the intensity distribution is calculated and absorption contributes to the carrier generation



- ✓ Reflection coefficients of top and bottom contacts,  $R_0$  and  $R_N$ , are directly specified by user
- ✓ Optical properties of each layer are calculated automatically from its composition using database of material properties

- ✓ **1D drift-diffusion model**
  - ✓ Poisson equation for the electric potential
  - ✓ Drift-diffusion carrier transport equations
  - ✓ Generation and recombination rates
- ✓ **Simulation of multi-cascade solar cells**
  - ✓ Tunnel junction characteristics can be either specified manually or computed by simulation of the band-to-band tunneling
- ✓ **Advanced numerical algorithms improve convergence and reduce computation time**



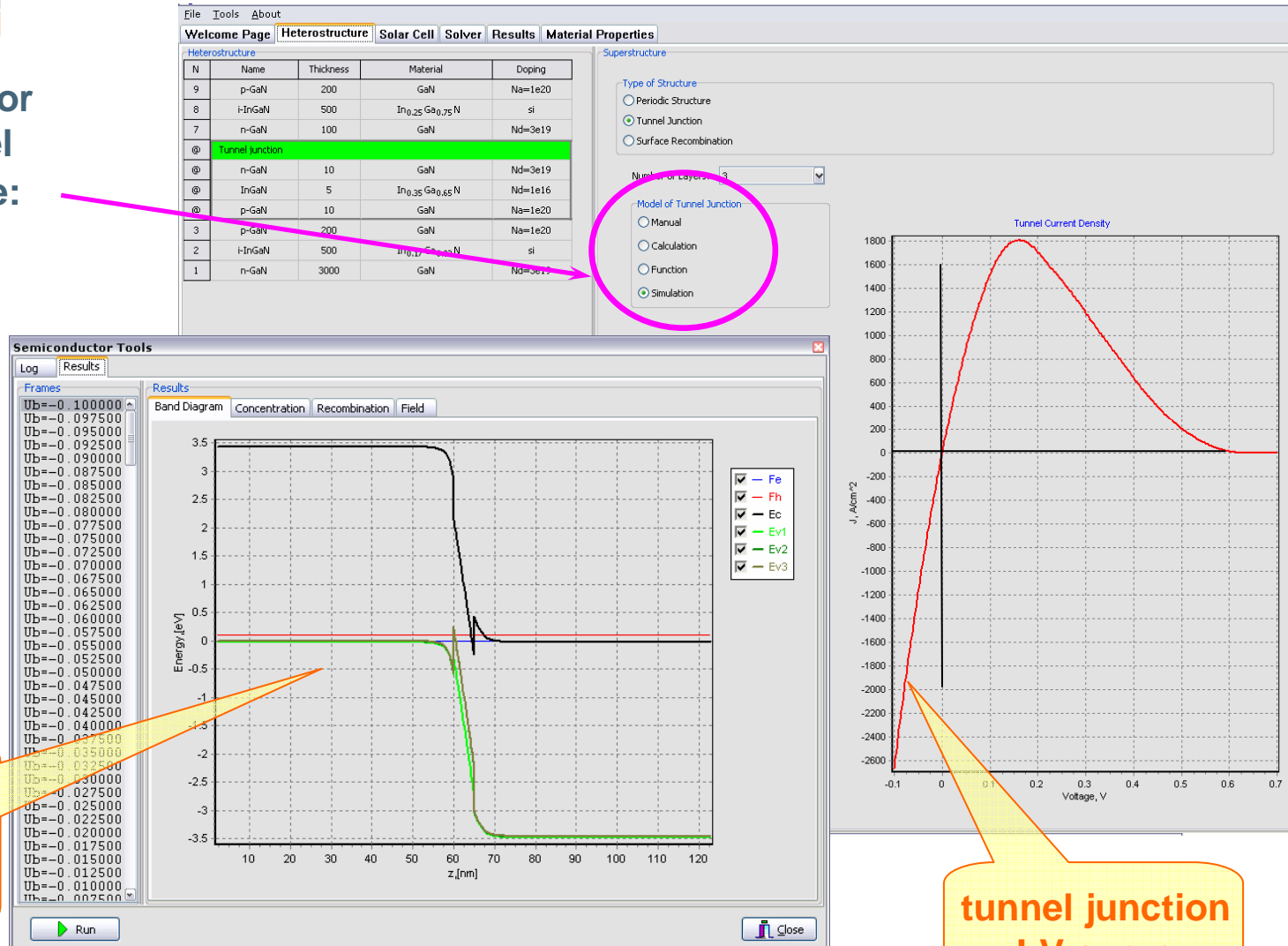


# Tunnel junction design and its characteristics

various options for calculating tunnel junction I-V curve:

- analytical (Kane model)
- experimental (table)
- WKB with account of interband transition

band diagrams of the tunnel junction at various biases



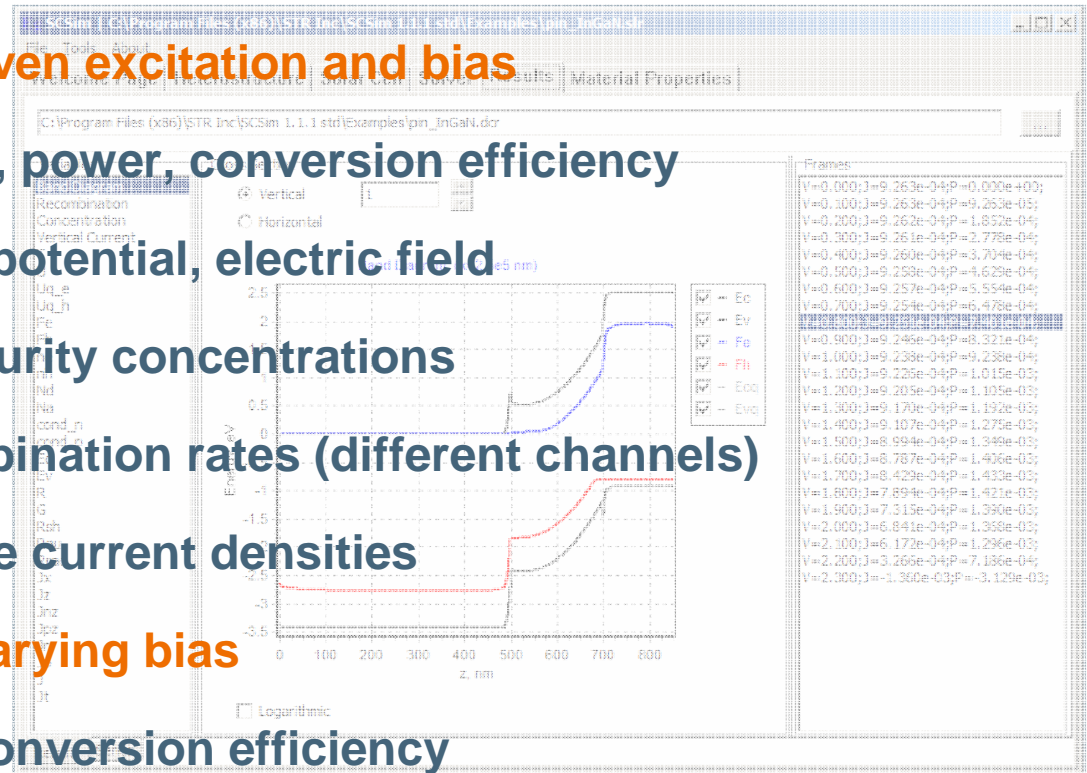
tunnel junction I-V curve



# Output parameters and characteristics

## ➤ Single computations at a given excitation and bias

- ✓ Current/current density, power, conversion efficiency
- ✓ Band diagram, electric potential, electric field
- ✓ Carrier and ionized impurity concentrations
- ✓ Generation rate, recombination rates (different channels)
- ✓ Partial electron and hole current densities



## ➤ Series computations with varying bias

- ✓ I-V characteristic and conversion efficiency
- ✓ Short-circuit current, open-circuit voltage, fill factor

## ➤ Series computations with varying excitation wavelength

- ✓ Spectral dependence of IQE and EQE

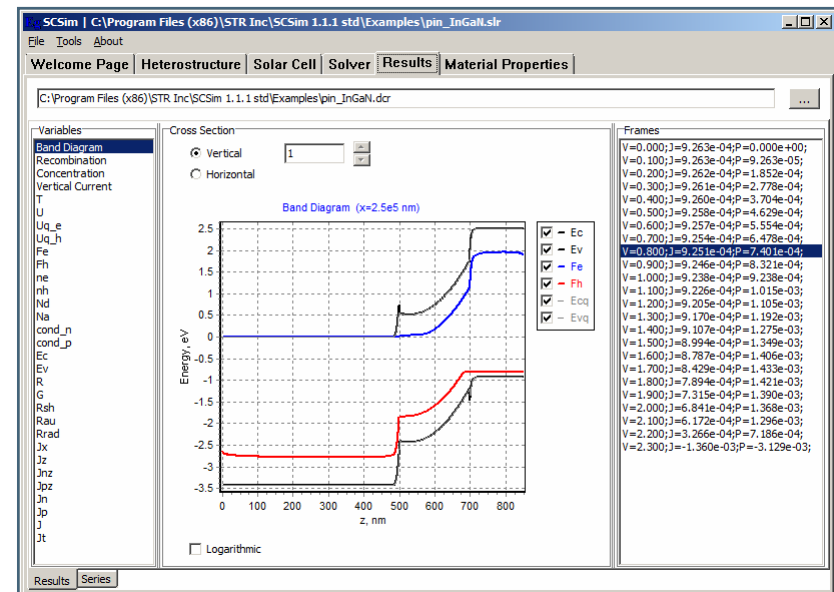




- ✓ Editable database of material properties
- ✓ Most of parameters can be specified as functional or tabulated dependencies on the temperature, wavelength, material composition, etc.
- ✓ Flexible specification of the excitation spectrum, including standard light sources, custom sources, monochromatic excitation.
- ✓ Built-in visualization of the simulation results

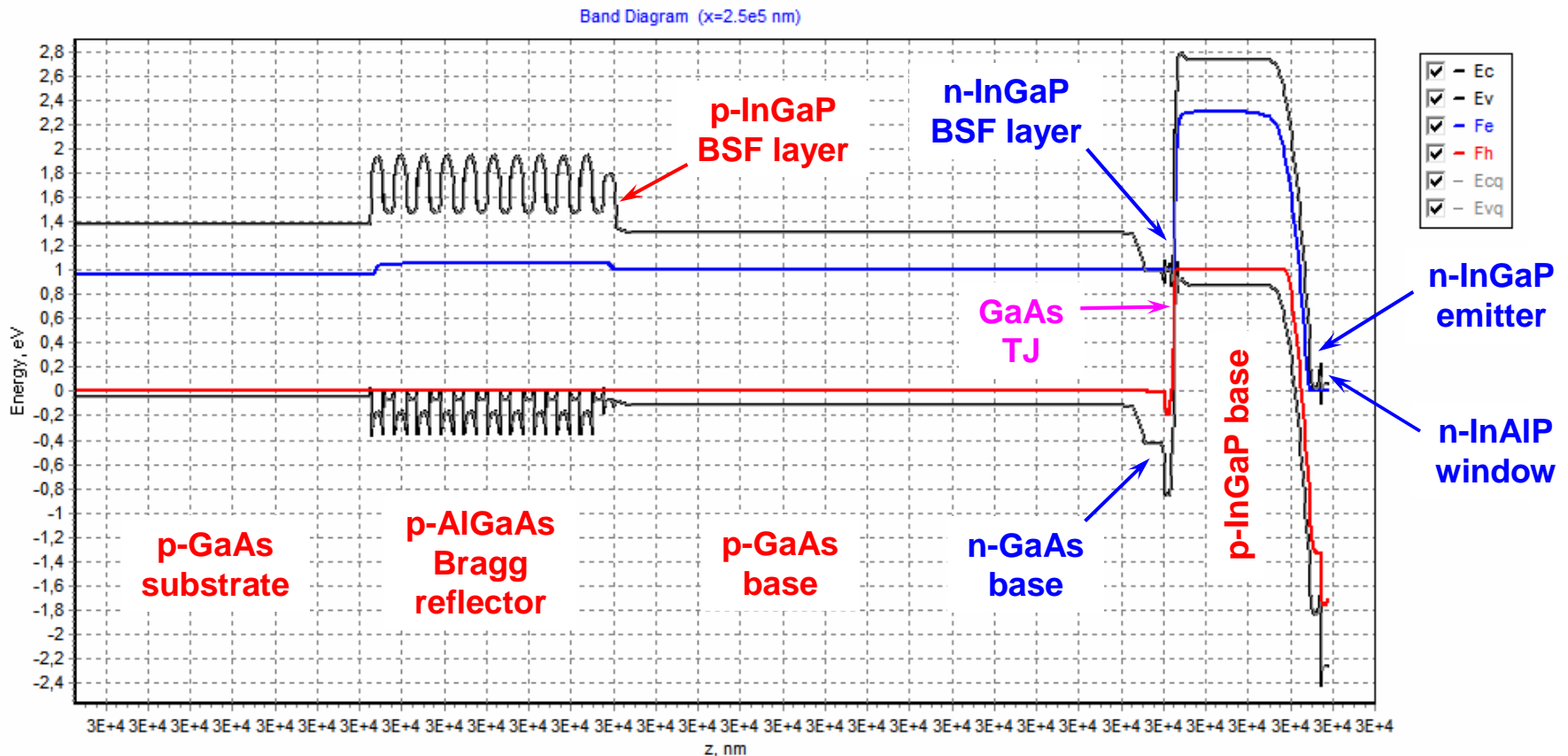
Learning time: ~ 3 days

Computation time: ~ 3 min





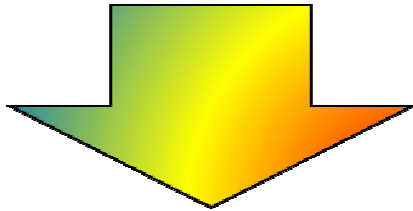
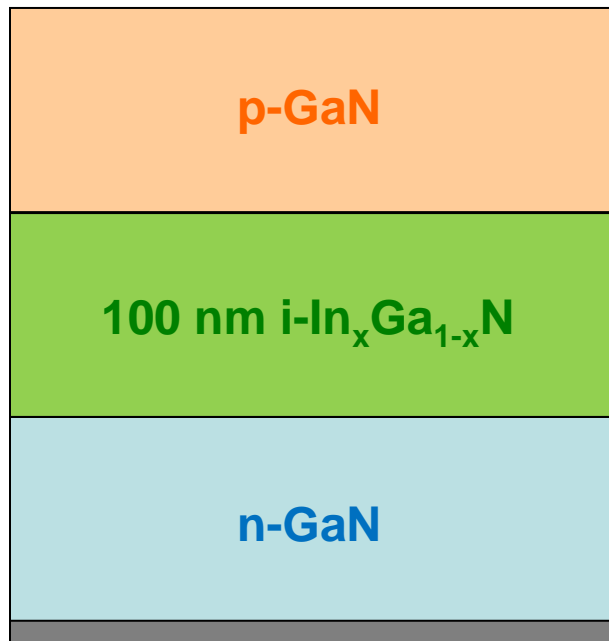
# Simulation of dual-junction GaInP-GaAs solar cell



analytical model for tunnel junction j-V characteristics is used; as a result, full simulation of the dual-junction solar cell has been performed within 1.5 min (no convergence was obtained for this structure by using an another software)



solar light

 $R = 0$  $R = 1$ 

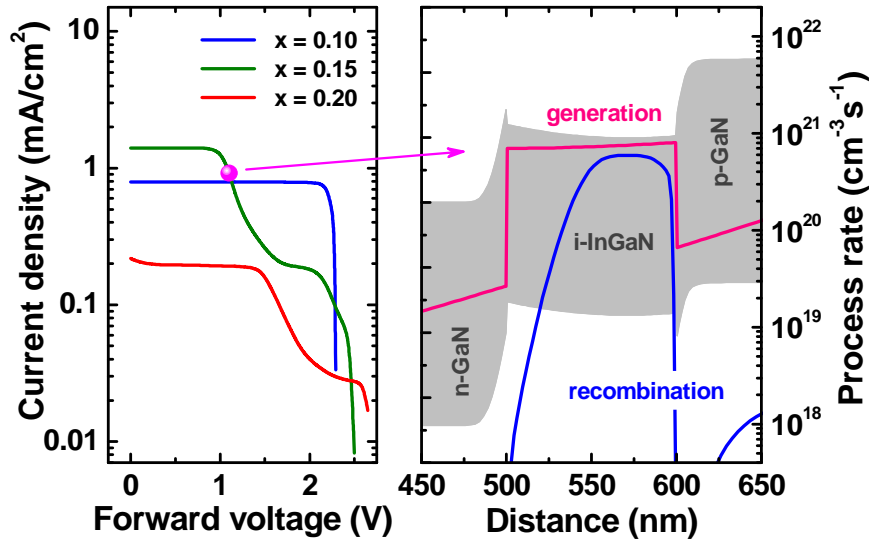
*Kirill A. Bulashevich and Sergey Yu. Karpov,  
Phys. Stat. Solidi (c) 11 (2014) 640*

Same electron and hole non-radiative carrier life time  $\tau$  in the InGaN active layer was chosen for the seek of simplicity. The effect of the carrier lifetime on the conversion efficiency has been also examined.

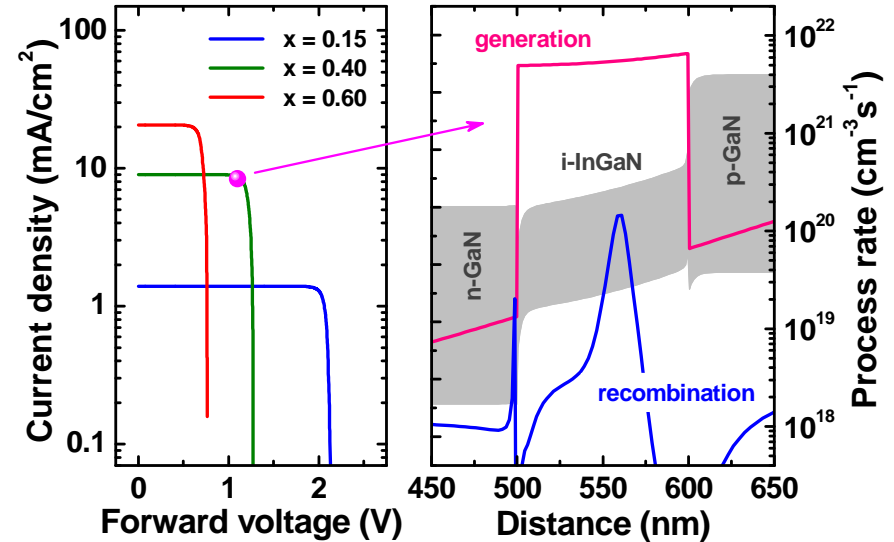
# Polarity effect on operation of strained solar cell structures



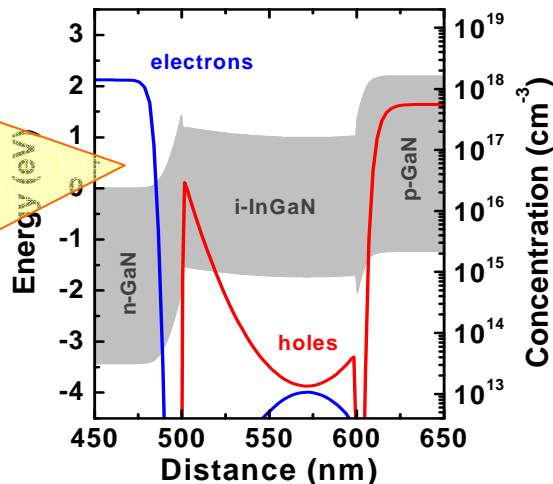
## III-polar structure



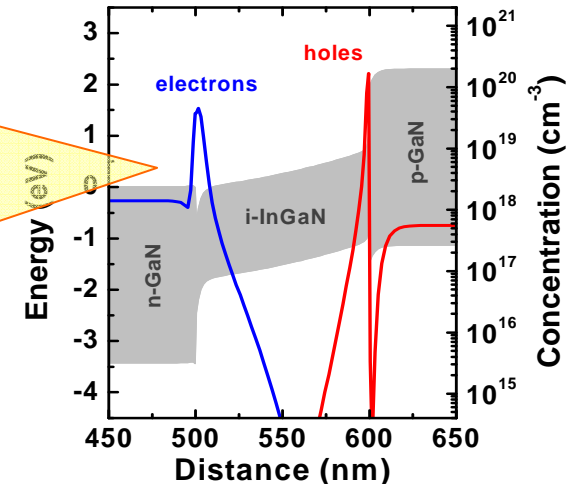
## N-polar structure



electric field in InGaN hinders separation of electrons and holes, making the structure inoperable at  $x > 0.20$



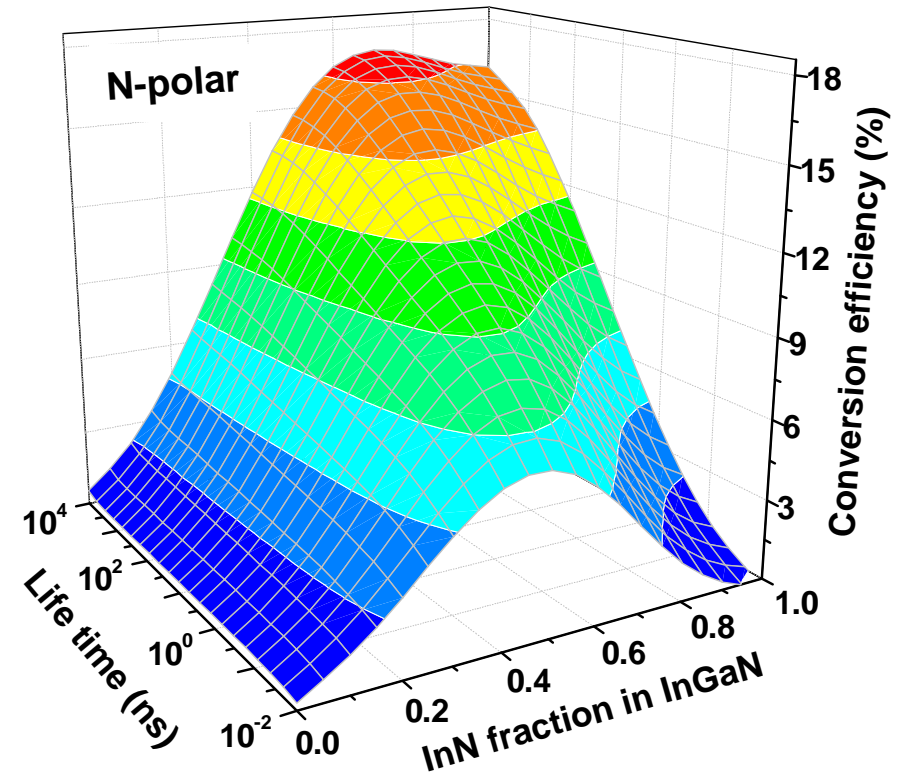
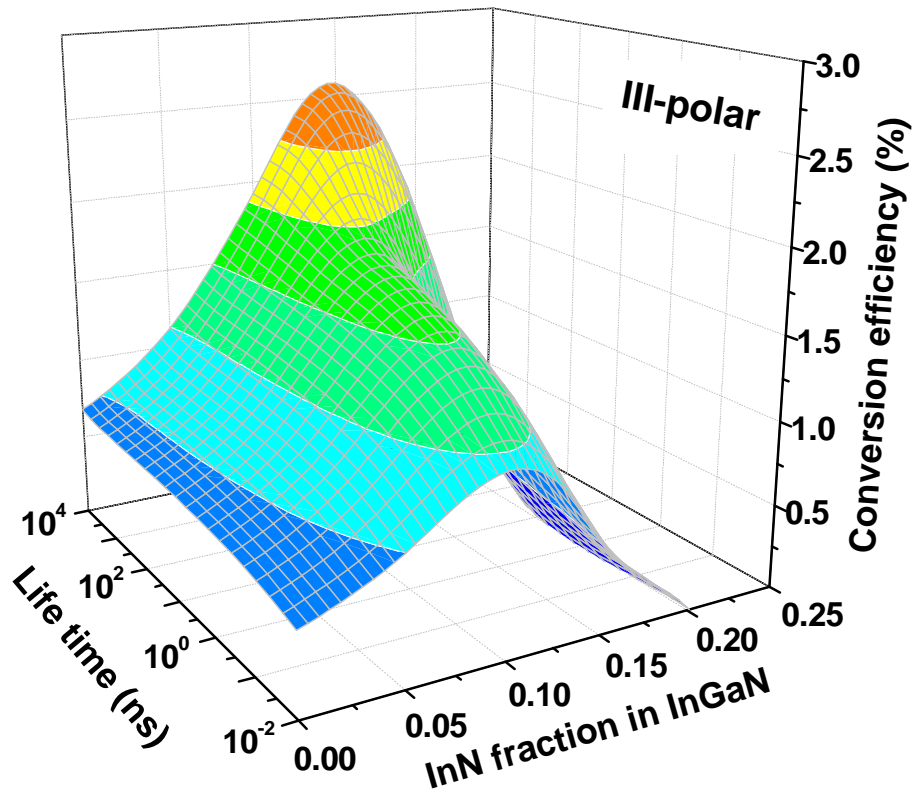
electric field in InGaN favors separation of electrons and holes at any alloy composition





# Conversion efficiency of strained solar cell structures

conversion efficiency at 1 sun (AM1.5G)



For both polarities, the conversion efficiency is limited by the absorptivity of the InGaN active layer corresponding to the optimal alloy composition, which does not exceed ~0.2 for III-polar structure.

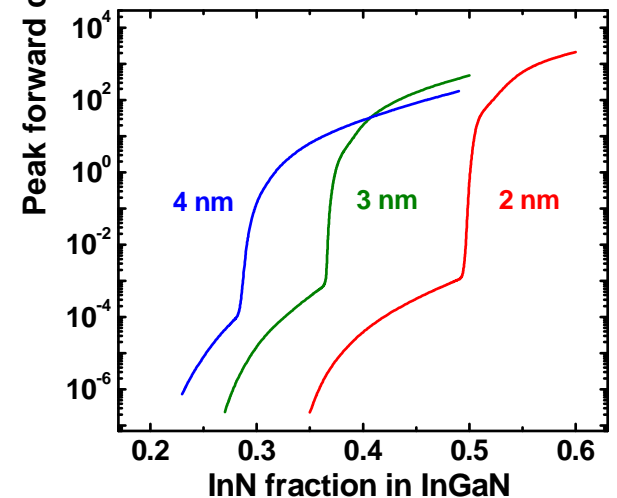
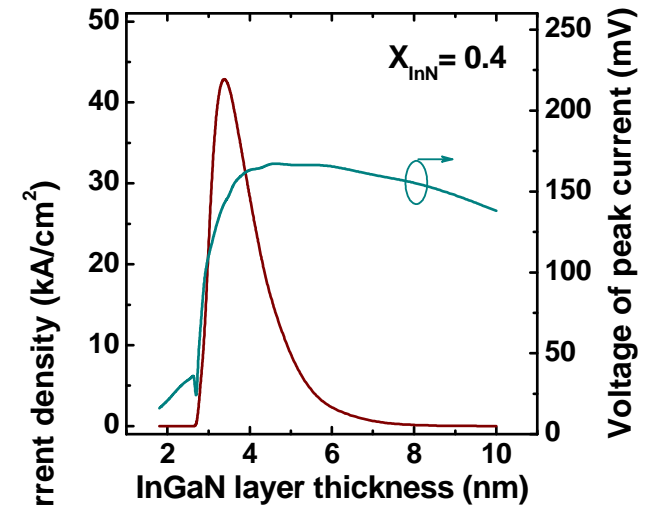
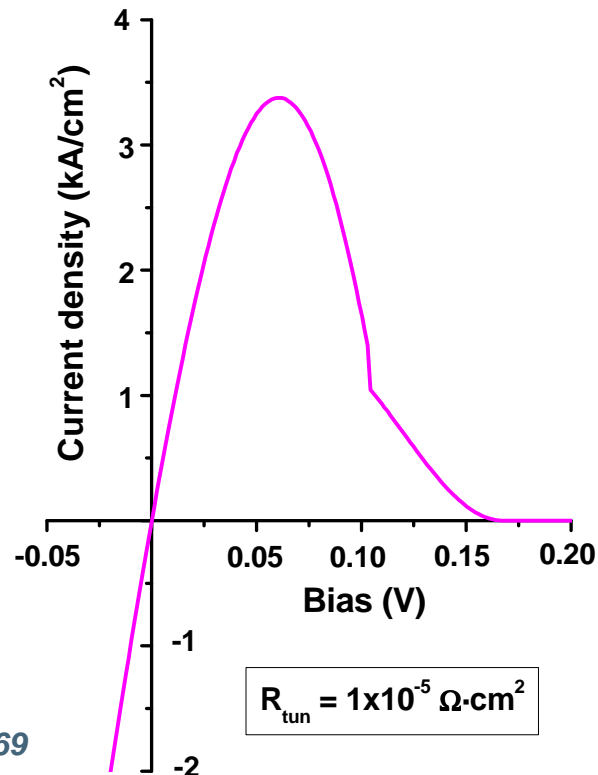
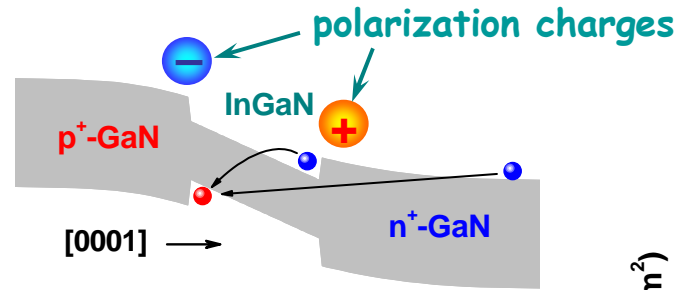
# Tunnel junction for III-nitride solar cells capable of forward-bias operation



Tunnel junctions in III-nitride solar cells should maintain high forward currents to provide a low junction resistance, which is impossible for the p-GaN/n<sup>+</sup>-GaN junctions because of limited hole concentrations

Using of polarization engineering may give solution of the problem

O.V. Khokhlev, K.A. Bulashevich, and S.Yu. Karpov,  
*Phys. Stat. Solidi (a)* 210 (2013) 1369





**PVcell** is the useful tool for design and optimization of semiconductor multijunction solar cells

**PVcell** software is supplied with

- Physics Summary
- GUI Manual
- Materials database
- Set of examples

Any questions on software operation and purchase procedure can be sent to [\*\*\*simuled-support@str-soft.com\*\*\*](mailto:simuled-support@str-soft.com)