

# SCAPS 3.0

## An introduction

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SCAPS 3.0

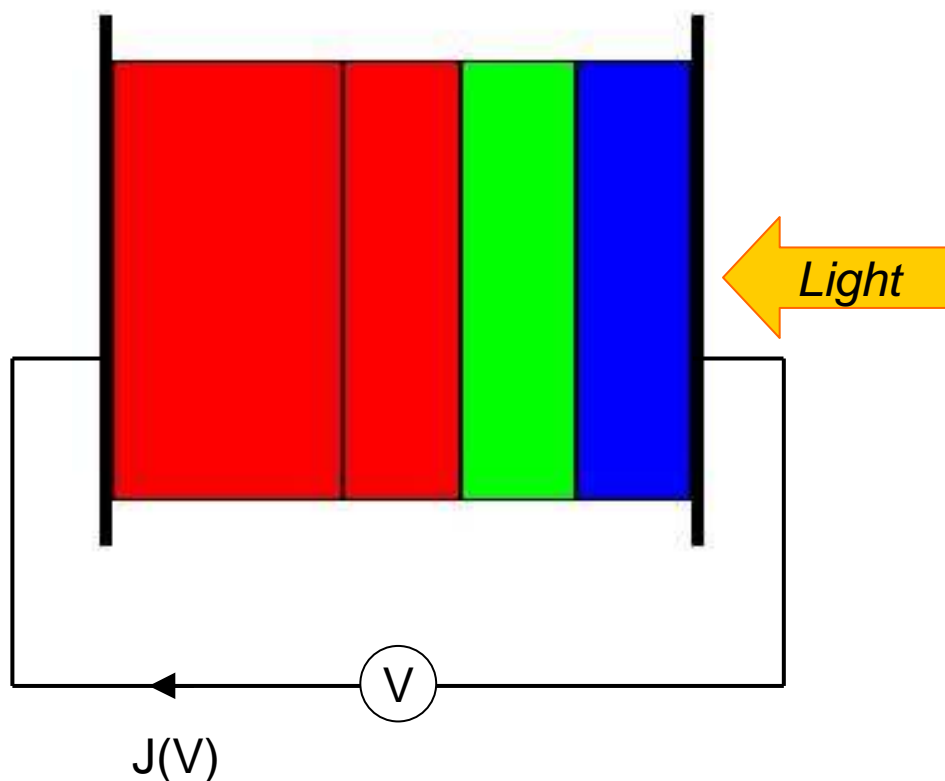
# Overview



- Getting started
- General working principles
- Tips & Tricks
  - Numerical limitations
  - The numerical panel
  - A neutral defect
  - Curve Info: *Get informed!*
  - Preserve your work for the future: *saving and commenting.*
  - Speeding up: *Batch – Recorder – Script*
  - Grading
  - Zooming: *Get a closer look!*
  - The blue button



# Getting Started...



- Opto-electrical simulation of **1-D structure** of semiconductor layers
- Special attention for contacts and interfaces
- Variable bias voltage, temperature & illumination
- DC & AC calculations
- Designed for CdTe and CIGS Solar Cells, but also used in other material systems 😊



# Getting Started

SCAPS 3.0 Action Panel

**Working point**  
 Temperature (K)   
 Voltage (V)   
 Frequency (Hz)   
 Number of points

**Series resistance**  
 yes  no  
 Rs: Ohm.cm<sup>2</sup>  Rsh  
 S/cm<sup>2</sup>  Gsh

**Shunt resistance**  
 yes  no

**Action list** — All SCAPS settings

1. Define Problem
2. Working Point
3. Select Calculations
4. Start Calculations
5. Analyze results

Illumination: Dark  Light  G(x): From internal SCAPS calculation  Reaction

**Light source for internal G(x) calculation**  
 Spectrum file:   
 Illuminated side: from  right (n-side)  left (p-side)  
 Incident (bias) light power (W/m<sup>2</sup>): sun or lamp   
 Spectrum cut off?  yes  no Short wavel. (nm)   
 Long wavel. (nm)   
 Neutral Dens.  Transmission (%)   
 after cut-off   
 after ND

**Action**  -Pause at each step

Action	V1 (V)	V2 (V)	f1 (Hz)	f2 (Hz)	WL1 (nm)	WL2 (nm)	number of points	increment
<input type="checkbox"/> Current voltage	<input type="text" value="0.0000"/>	<input type="text" value="0.8000"/>					<input type="text" value="41"/>	<input type="text" value="0.0200"/> increment (V)
<input type="checkbox"/> Capacitance voltage	<input type="text" value="-0.8000"/>	<input type="text" value="0.8000"/>					<input type="text" value="81"/>	<input type="text" value="0.0200"/> increment (V)
<input type="checkbox"/> Capacitance frequency			<input type="text" value="1.000E+2"/>	<input type="text" value="1.000E+6"/>			<input type="text" value="21"/>	<input type="text" value="5"/> points per decade
<input type="checkbox"/> Spectral response					<input type="text" value="300"/>	<input type="text" value="900"/>	<input type="text" value="61"/>	<input type="text" value="10"/> increment (nm)

**Set problem** loaded definition file:  Problem file:  Set Problem

**Calculate: single shot** **Calculate: batch** **Calculate: recorder** **Execute script**

**Continue** **Stop**

**Batch set-up** **Record set-up** **Script set-up**

**Results of calculations**  
 EB  G,R  AC  I-V  G-V  C-F  QE

**Recorder results**  
 Script graphs

**Save all simulations** **Clear all simulations**

**SCAPS info** **Quit**



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# Getting Started: Define Problem

- Setting Layer, Interface & Contact properties
- Setting Numerical preferences
- Saving & Loading



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SCAPS 3.0.0 Layer Properties Panel

LAYER 1 CISSe

thickness ( $\mu\text{m}$ ) 1.800

Layer Composition GradingType **uniform y,  $0 < y < 1$**

Uniform composition y = 0.100 0.100

Semiconductor Property P of the pure materi:	pure A (y = 0)	pure B (y = 1)	Composition dependence
bandgap (eV)	1.040	1.530	parabolic
electron affinity (eV)	4.300	4.300	uniform
dielectric permittivity (relative)	12.000	12.000	uniform
CB effective density of states ( $1/\text{cm}^3$ )	$7.000\text{E}+17$	$7.000\text{E}+17$	uniform
VB effective density of states ( $1/\text{cm}^3$ )	$1.500\text{E}+19$	$1.500\text{E}+19$	uniform
electron thermal velocity ( $\text{cm}/\text{s}$ )	$1.000\text{E}+7$	$1.000\text{E}+7$	uniform
hole thermal velocity ( $\text{cm}/\text{s}$ )	$8.000\text{E}+6$	$8.000\text{E}+6$	uniform
electron mobility ( $\text{cm}^2/\text{Vs}$ )	$1.000\text{E}+2$	$1.000\text{E}+2$	uniform
hole mobility ( $\text{cm}^2/\text{Vs}$ )	$2.500\text{E}+1$	$2.500\text{E}+1$	uniform
effective mass of electrons	$1.000\text{E}+0$	$1.000\text{E}+0$	uniform
effective mass of holes	$1.000\text{E}+0$	$1.000\text{E}+0$	uniform

ND grading dependent: on composition y: ND (y)  Allow Tunneling

shallow donor density ND(y) ( $1/\text{cm}^3$ )  $1.000\text{E}+5$   $1.000\text{E}+5$  uniform

NA grading dependent: on composition y: NA (y)

shallow acceptor density NA(y) ( $1/\text{cm}^3$ )  $5.000\text{E}+15$   $5.000\text{E}+15$  uniform

Absorption model **Show /Set alpha(composition; lambda)**

	alpha (y=0)	alpha (y=1)
absorption constant A ( $1/\text{cm eV}^2$ )	$1.000\text{E}+5$	$1.000\text{E}+5$
absorption constant B ( $\text{eV}^2/\text{cm}$ )	$0.000\text{E}+0$	$0.000\text{E}+0$

from model from file from model from file

CISMöller.abs CuInS2\_Alonso\_Mölle

absorption file for y = 0 absorption file for y = 1

Recombination model

Band to band recombination

Radiative recombination coefficient ( $\text{cm}^3/\text{s}$ )	$0.000\text{E}+0$	$0.000\text{E}+0$	uniform
Auger hole capture coefficient ( $\text{cm}^6/\text{s}$ )	$0.000\text{E}+0$	$0.000\text{E}+0$	uniform
Auger hole capture coefficient ( $\text{cm}^6/\text{s}$ )	$0.000\text{E}+0$	$0.000\text{E}+0$	uniform

Recombination at defects

Defect 1

charge type : acceptor : {0/}

total density ( $1/\text{cm}^3$ ): Uniform  $1.000\text{E}+16$

grading Nt(x): uniform

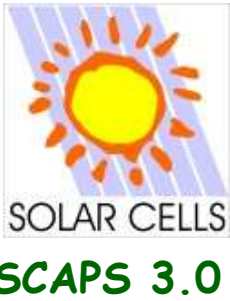
energydistribution: single; Et = 0.40 eV above EV

this defect only, if active: tau\_n =  $1.0\text{e}+00$  ns, tau\_p =  $1.3\text{e}+01$  ns

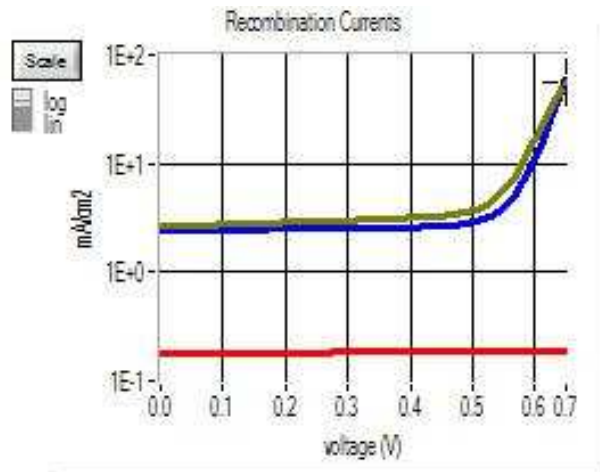
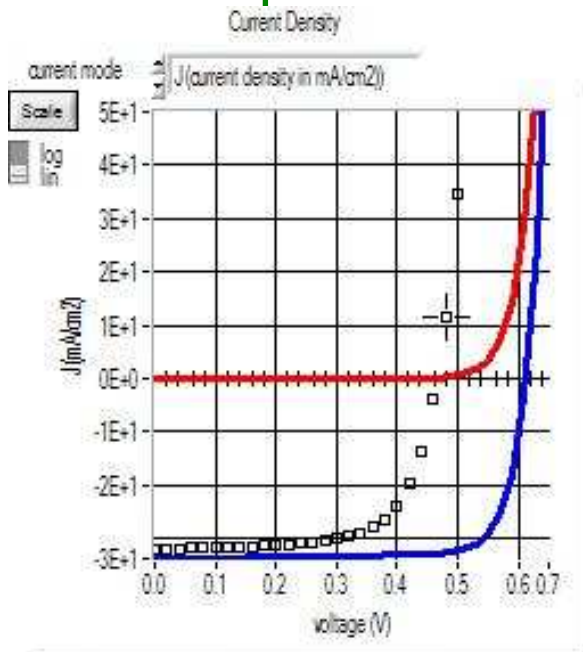
this defect only, if active: Ln =  $5.1\text{e}-01$   $\mu\text{m}$ , Lp =  $9.0\text{e}-01$   $\mu\text{m}$

none

Accept cancel



# Getting Started: Analyze results



Last simulated IV parameters			
Voc(V)	Jsc(mA/cm²)	FF (%)	eta (%)
0.6124	33.746271	79.80	16.49
Measured IV parameters			
0.4655	32.100000	67.35	10.06

Total recombination:  
 At front contact  
 At back contact  
 At interface  
 In semiconductors  
 total SRH  
 total recombination  
 total Auger

Measurement file:  
 File name: c:\Koen\Scaps\SCAPS 21003\werkuerse\measurements\Numos Ex 1 light.iv

Curve info

- Display results
- Export results
- Compare with measured data
- Navigate to other panels

last curve. <-light  
 Problem file: c:\Koen\Scaps\SCAPS 21003\werkuerse\def\Numos CIGS baseline.def  
 last saved: 22-3-2007 at 19:30:28  
 simulation done on: 11-2-2011 at 12:4:50



General working principles:

# Semiconductor equations



$$\left[ \frac{\partial}{\partial x} \left( \epsilon \frac{\partial \psi}{\partial x} \right) = -\frac{q}{\epsilon_0} \left[ -n + p - N_A^- + N_D^+ + \frac{1}{q} \rho_{defect}(n, p) \right] \right] \quad \text{Poisson}$$

$$\left. \begin{cases} -\frac{\partial j_n}{\partial x} + G - U_n(n, p) = \frac{\partial n}{\partial t} \\ -\frac{\partial j_p}{\partial x} + G - U_p(n, p) = \frac{\partial p}{\partial t} \end{cases} \right\} \quad \text{Continuity relations}$$

Constitutive relations

$$\begin{cases} j_n = -\frac{\mu_n}{q} n \frac{\partial E_{Fn}}{\partial x} \\ j_p = \frac{\mu_p}{q} p \frac{\partial E_{Fp}}{\partial x} \end{cases}$$

- Boundary conditions at interfaces and contacts
- RESULT: system of coupled differential equations in  $\{\psi, n, p\}$  or  $\{\psi, E_{Fn}, E_{Fp}\}$
- Solved numerically



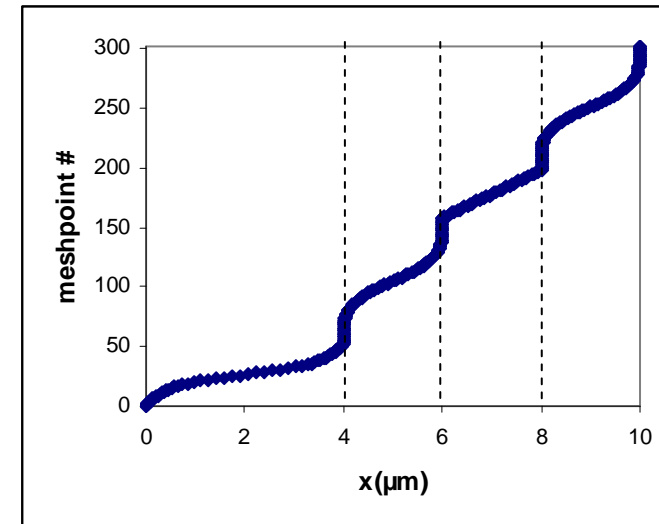
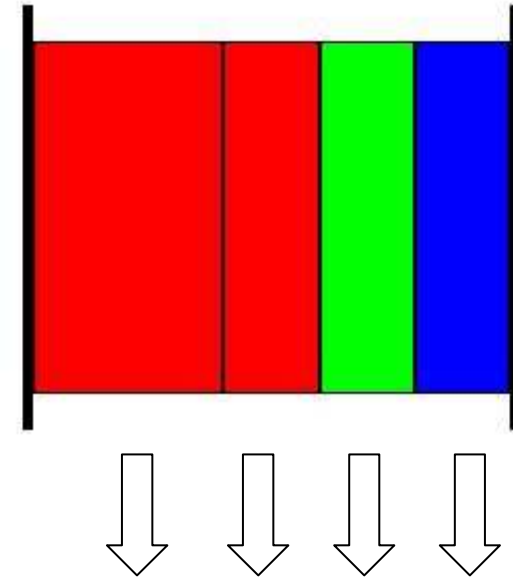


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General working principles:

# Discretization

- Equations solved using finite differences
- Structure discretized => MESH
  - Coarse meshing in the middle of a layer
  - Finer mesh near the interfaces & contacts
  - Two discretization points for each interface
  - Meshing can be updated during simulation process (numerical panel)





General working principles:

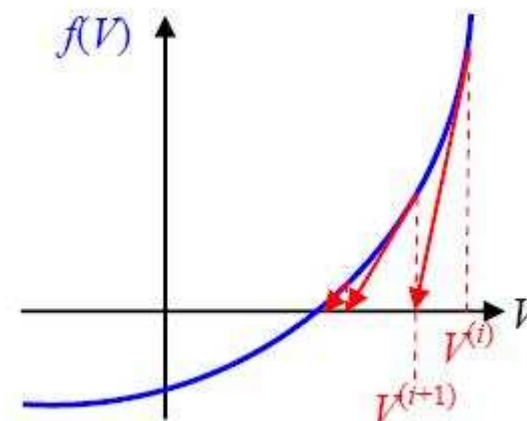
# The pathway to a solution<sup>1</sup>



¿Gummel scheme with Newton Raphson substeps?

- Solve (1) for  $\psi$  with given  $E_{Fn}$  &  $E_{Fp}$
- Solve (2) for  $E_{Fn}$  with given  $\psi$  &  $E_{Fp}$
- Solve (3) for  $E_{Fp}$  with given  $\psi$  &  $E_{Fn}$

$$\left\{ \begin{array}{l} (1): \frac{\partial}{\partial x} \left( \epsilon \frac{\partial \psi}{\partial x} \right) = -\frac{q}{\epsilon_0} \left[ -n + p - N_A^- + N_D^+ + \rho_{defect}(n, p) \right] \\ (2): -\frac{\partial j_n}{\partial x} + G - U_n(n, p) = \frac{\partial n}{\partial t} \\ (3): -\frac{\partial j_p}{\partial x} + G - U_p(n, p) = \frac{\partial p}{\partial t} \end{array} \right.$$

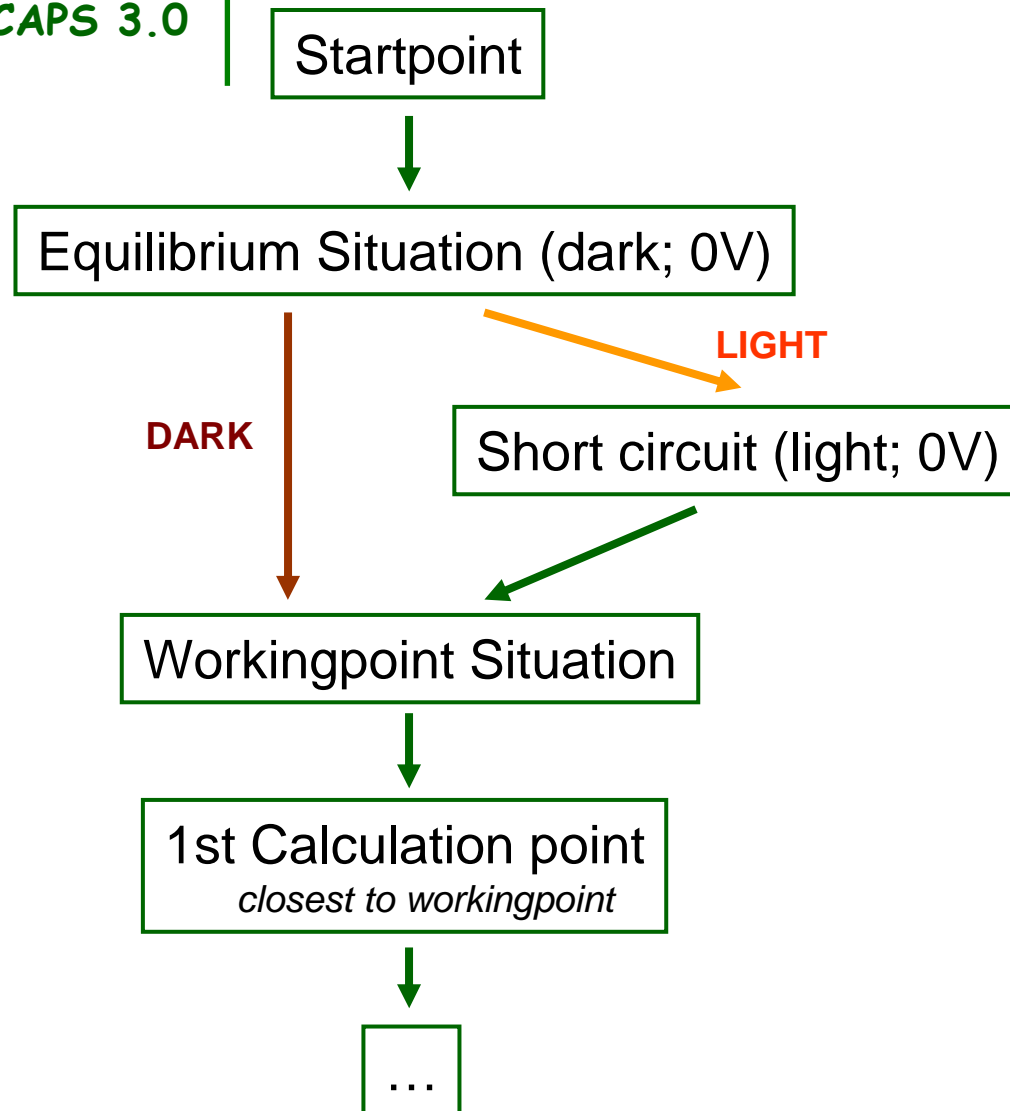


- Make first guess of solution
- Improve guess with tangent lines
- Works well if first guess was not too bad



General working principles:

# The pathway to a solution<sup>2</sup>



- Difference between several steps should not be too large
- Number of intermediate steps to get to the workingpoint can be set
- Every batch step starts at the startpoint



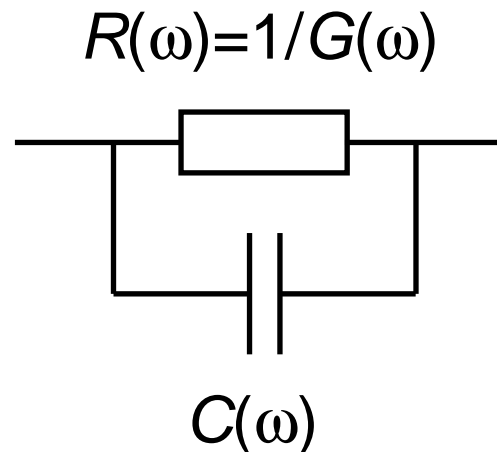
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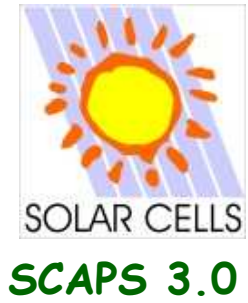
General working principles:

# AC-analysis

- Small signal analysis:  $\tilde{V} \rightarrow 0$
- Small signal values are complex numbers!!!
- Small signal currents, potential ( $\psi$ ) and Fermi levels displayed on ac-panel
- Admittance interpreted as capacitance-conductance circuit

$$\begin{cases} V = V_{DC} + \tilde{V}e^{j\omega t} \\ \psi = \psi_{DC} + \tilde{\psi}e^{j\omega t} \\ E_{Fn} = E_{Fn,DC} + \tilde{E}_{Fn}e^{j\omega t} \\ j_n = j_{n,DC} + \tilde{j}_n e^{j\omega t} \end{cases}$$





# Tips and Tricks





# Numerical limitations

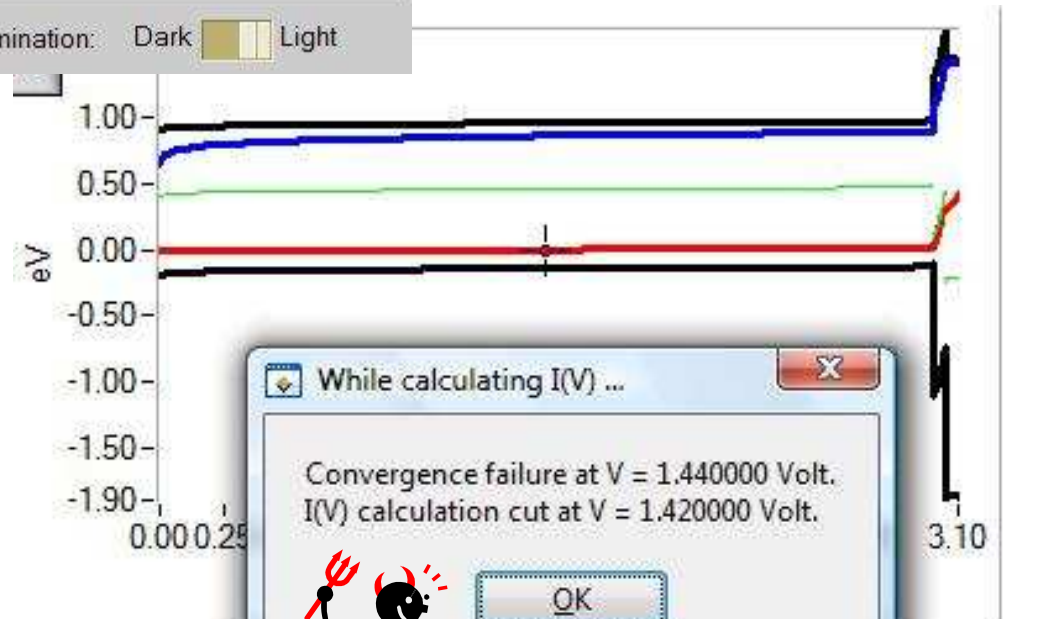
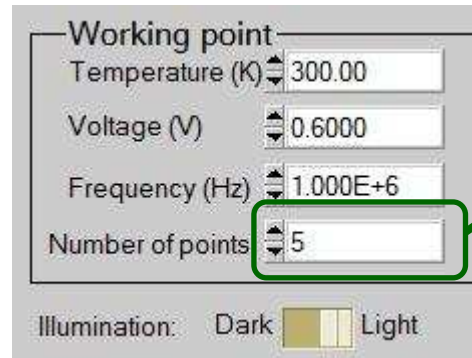
- Keep the variation between different calculation steps limited.
- Keep it realistic: SCAPS is developed and tested to simulate realistic situations, hence things can go wrong when simulating unphysical situations
- Don't overdo  
Do you really want to know the current at  $T=20K$ ,  $V=300V$ ?
- Stop after  $V_{oc}$   
Don't calculate the strong forward currents (slow to calculate) if you don't need them.

Stop after Voc

Large number of points:

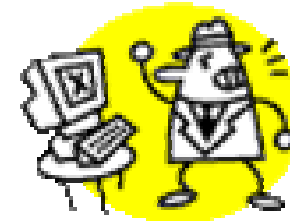
→ Slower calculation

→ Less chance of convergence failure





# Numerical limitations

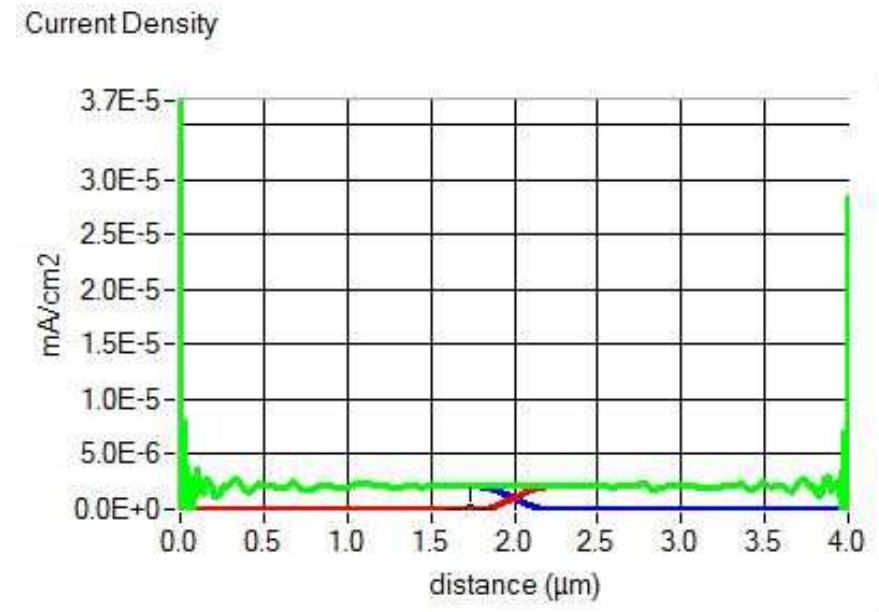
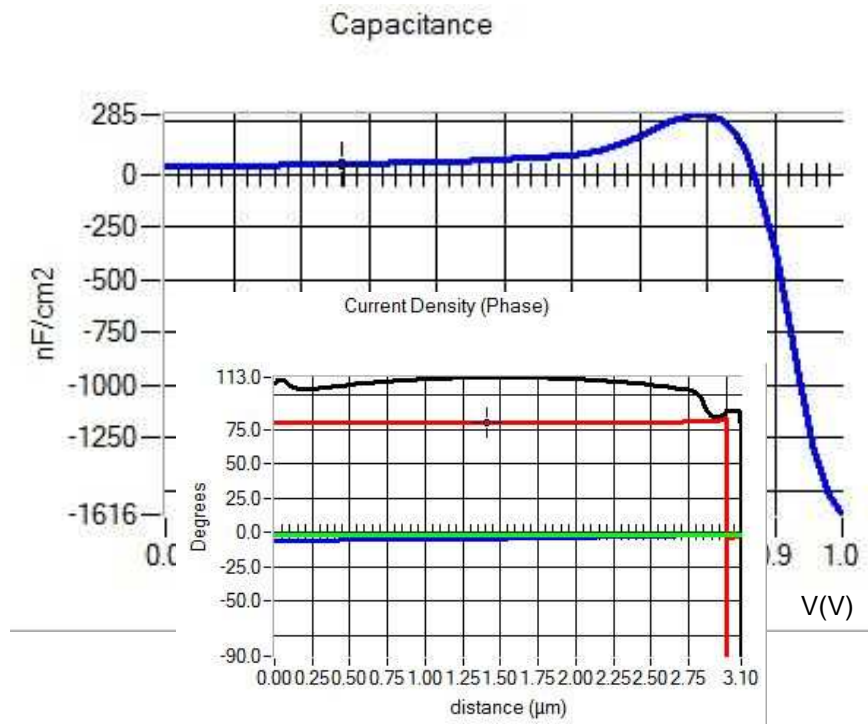


$$1.000 - 10^{-15} \neq 1.000$$

AC-calculation when  $\text{Re}(J) \gg \text{Im}(J)$

- negative capacitances
- $C$  increases with frequency

$pn \leftrightarrow np$ -structure





# The numerical panel<sup>1</sup>

Avoid too big variations between iterations

Terminations criteria  
Newton-Raphson

**Convergence settings**

maximum number of iterations:

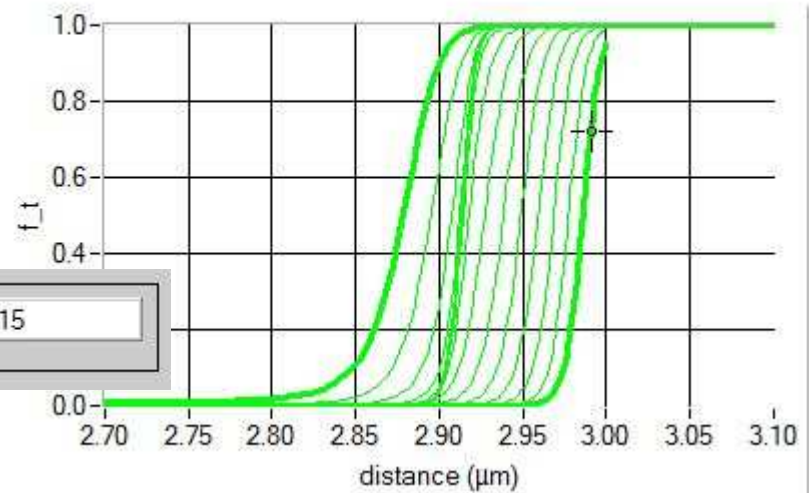
maximum variation (kT/q):

$\psi$	electrostatic potential	per iteration (clamp): <input type="text" value="0.50"/>	last iteration (termination criterion): <input type="text" value="1.0E-3"/>
$E_{Fn}$	electron Fermi level	<input type="text" value="0.50"/>	<input type="text" value="1.0E-3"/>
$E_{Fp}$	hole Fermi level	<input type="text" value="0.50"/>	<input type="text" value="1.0E-3"/>

Convergence failure messages:

Output list after a convergence failure:

Occupation probability of deep defects for electrons [SCAPS 2.8 and earlier]



number of discretization levels for distributed defects:

Plot all occupation levels





# The numerical panel<sup>2</sup>

**Mesh generator settings**

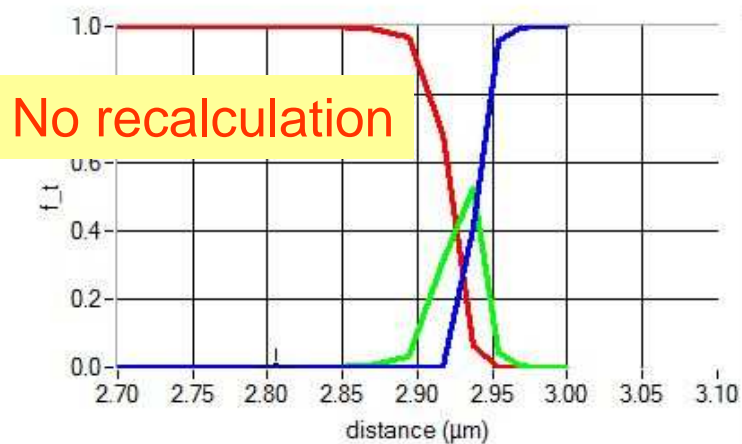
Recalculate the mesh during iterations

maximum ratio between neighbouring mesh points	1.60
minimum ratio between neighbouring mesh points	1.05
generation limit (microAmps/cm <sup>2</sup> )	1.00E+0
recombination limit (microAmps/cm <sup>2</sup> )	1.00E-3

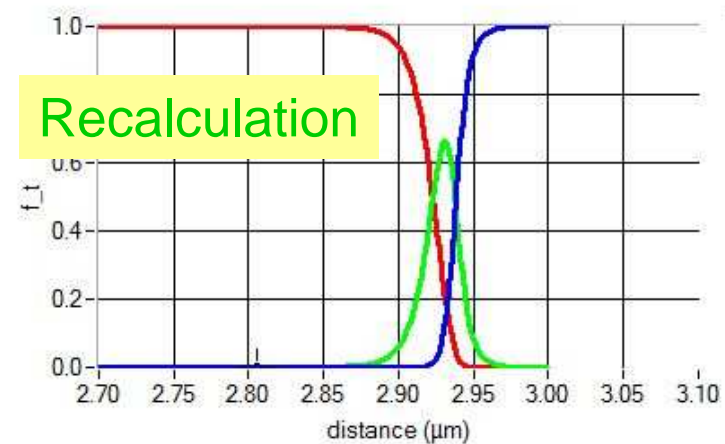
Remove/add mesh points:  
based on:

- $\psi$ ,  $E_{Fn}$  and  $E_{Fp}$
- Generation
- Recombination

Occupation probability of deep defects:  
Charge distribution



Occupation probability of deep defects:  
Charge distribution



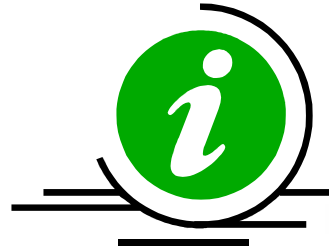


## A Neutral Defect

- Recombination present  $\leftrightarrow$  No influence on charges
  - Separation of direct and charge related effects of defects
- Does not exist in real materials
- Handy in simulation
  - Whilst building model
  - For unimportant layers
- Neutral defect + shallow doping  $\sim$  charged defect



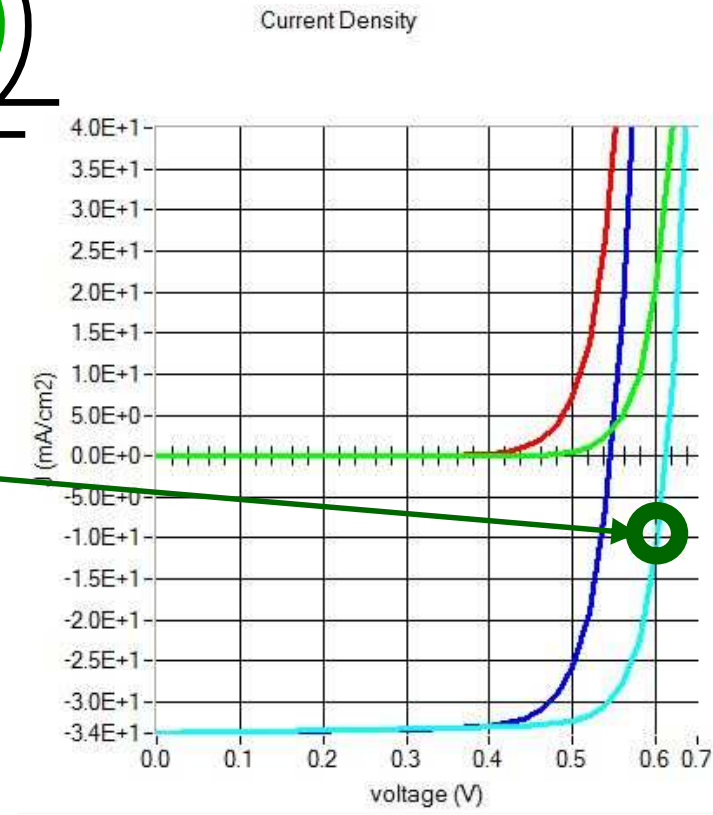
# Curve Info



graph: J-V curve: J(V)  
(lin-lin plot)

curve: Batch simulation 1: 2 param., step 4/4  
temperature [K]: 3.000e+02  
illumination>>dark?: 0.000e+00  
---

point: point # 30  
6.0000e-01 voltage (V)  
-1.1543e+01 J (mA/cm2)



- Information about Graph/Curve/Point when clicking on a plot:
- Point/Curve nearest to mouse-click selected.
- ¿ Which curve corresponds to which simulation?



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# Save your work and settings

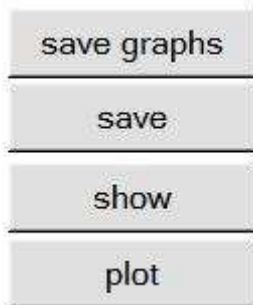
- Save settings:

- Cell structure (.def)  
[some of the numerical settings are included here]
- Batch (.sbf & .bdf)
- Recorder (.srf)
- Action panel (.act)



All together (.scaps)

- Save results:

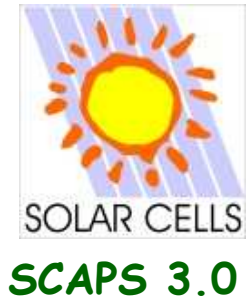


- To figure format (.png/.jpg/.bmp)
- To text file (or .xls-file)
- To screen
- To printer (or pdf-printer)



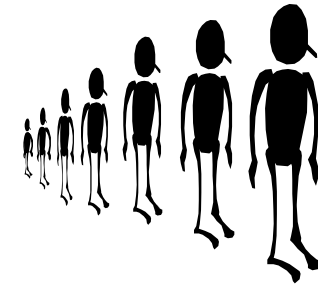
All files can be read with a text editor

• **ADDING COMMENT STRONGLY RECOMMENDED!**



Speeding up:

# Batch



Parameters varied simultaneously

Vary entire definition files

- Linear variation
- Logarithmic variation
- Custom defined variation

Simultaneous

Remove	p-CGS (L1)	defect 1	total defect de	left side	From: 1.000E+15	To: 1.000E+16	Steps: 7	Custom list: Lin <input checked="" type="checkbox"/> Log <input type="checkbox"/>
Remove	<input type="checkbox"/> n-CdS (L2)	thickness[ $\mu\text{m}$ ]			0.100	0.150	2	Lin <input type="checkbox"/> Log <input type="checkbox"/>
Remove	<input checked="" type="checkbox"/> n-ZnO (L3)	thickness[ $\mu\text{m}$ ]			0.250	0.150	2	Lin <input type="checkbox"/> Log <input type="checkbox"/>
Remove	<input type="checkbox"/> T [K]							
Remove	<input type="checkbox"/> illumination...	Spectrum file						3 values saved in three temperatures.bdf <input checked="" type="checkbox"/>


file as parameter!

Set custom values

Set Set

unsaved list of 2 spectrum files

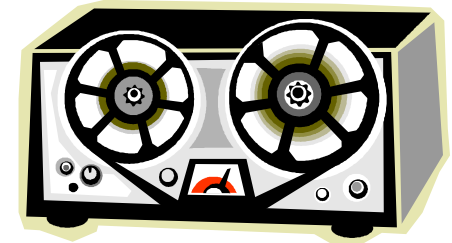
Up to 9 parameters

 Keep SHIFT pressed to interrupt a batch calculation

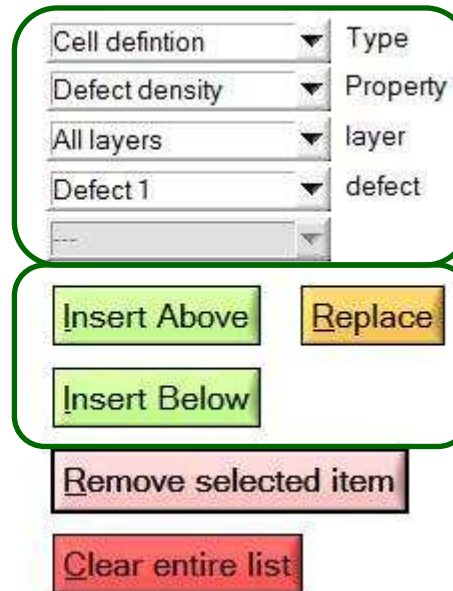
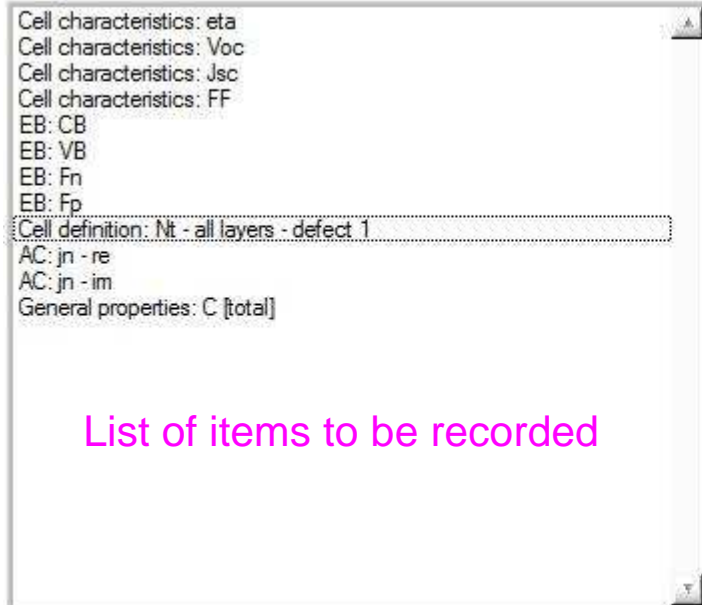


Speeding up:

# Recorder<sup>1</sup>



Properties to be recorded

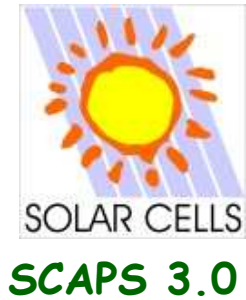


1. Select item to be recorded

2. Press to add to the list

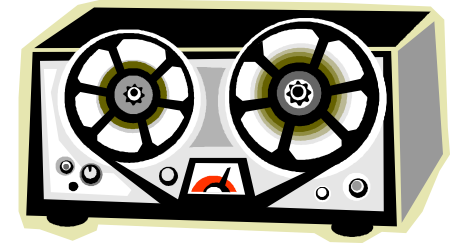


- The recorder overrules all calculations set at the action panel
- Items recorded at workingpoint conditions
- Only simulations to get to the asked properties are performed



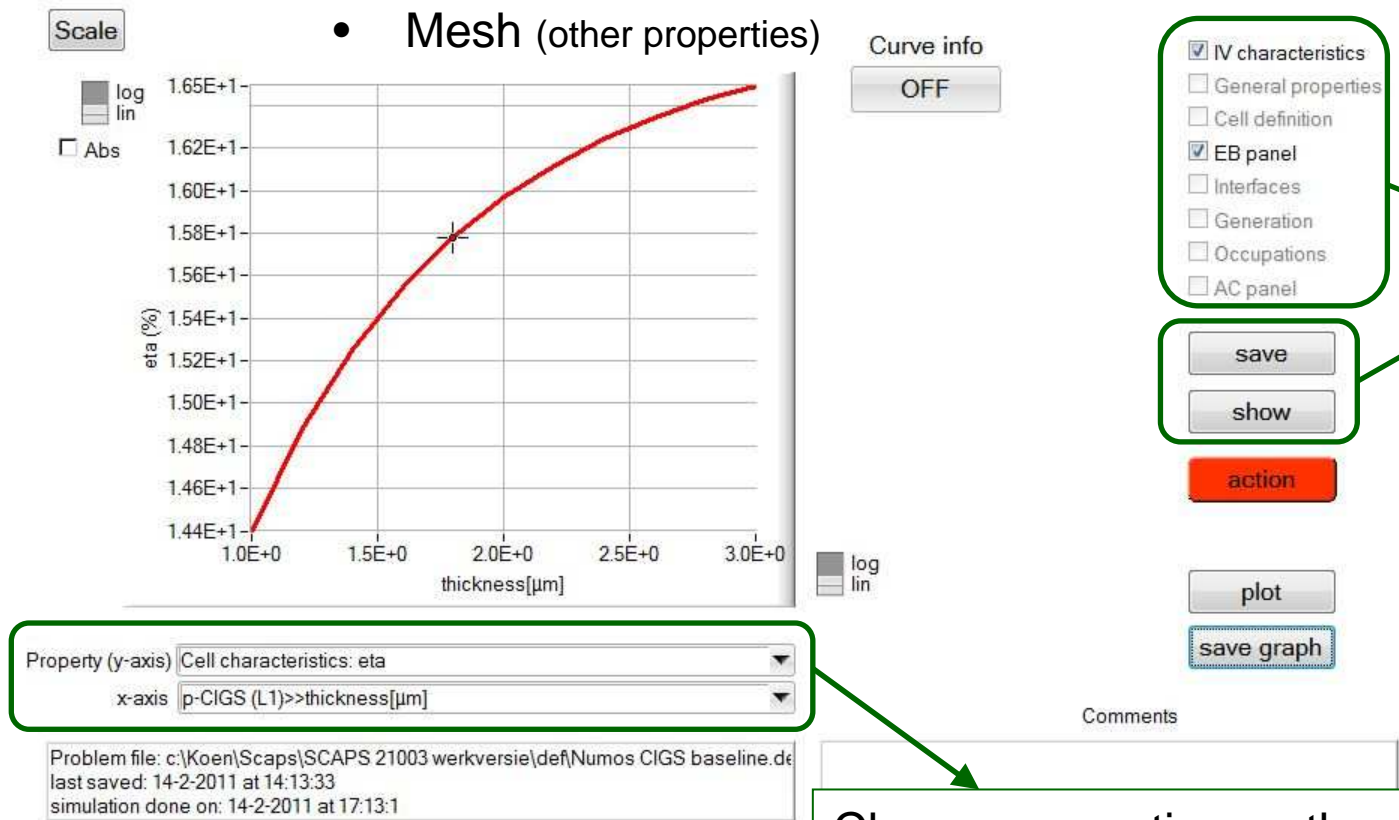
Speeding up:

# Recorder<sup>2</sup>



Recorded items shown as function of:

- Batch parameters (cell characteristics – general properties – interface properties)
- Mesh (other properties)



- Only checked items are saved
- Only lowest checked item is shown

Choose properties on the axes



Speeding up:

# Script



- Run *SCAPS* from command-line or external program
- Automate user-interface operations
- Analyze results in a non standard way
  - Make your own extension to *SCAPS*: `SCAPSUserFunction.dll`
  - Root/extrema finding available
  - Access all recordable variables: `singleshotbatch`



- Keep the script manual close at hand
- Freedom has its price! While scripting you have more power to let things go wrong





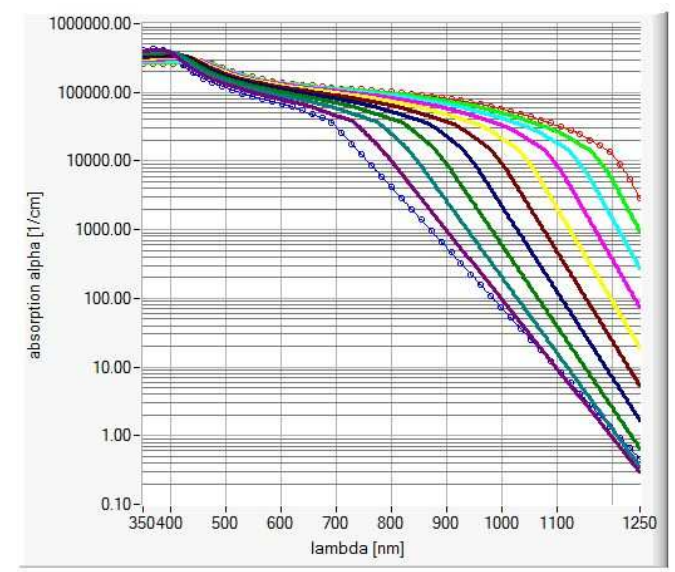
SCAPS 3.0

# Grading

ND grading dependent on position x: ND (x)			
shallow donor density ND(x) (1/cm3)	1.000E+15	1.000E+16	parabolic
NA grading dependent: on composition y: NA (y)			
shallow acceptor density NA(y) (1/cm3)	1.000E+1	1.000E+17	exponential

- Material driven approach
- $N_A$ ,  $N_D$ ,  $N_T \rightarrow$  Grading along **composition** or **position**
- What is UNIFORM?
  - **Uniform A / Uniform B**: Only one material present (nothing else can/should be graded)
  - **Uniform Y**: Uniform material is a mixture of two materials (other parameters can be graded)
- Special absorption interpolation

Graded variables available on the cell definition panel after calculation

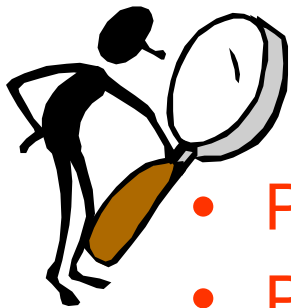
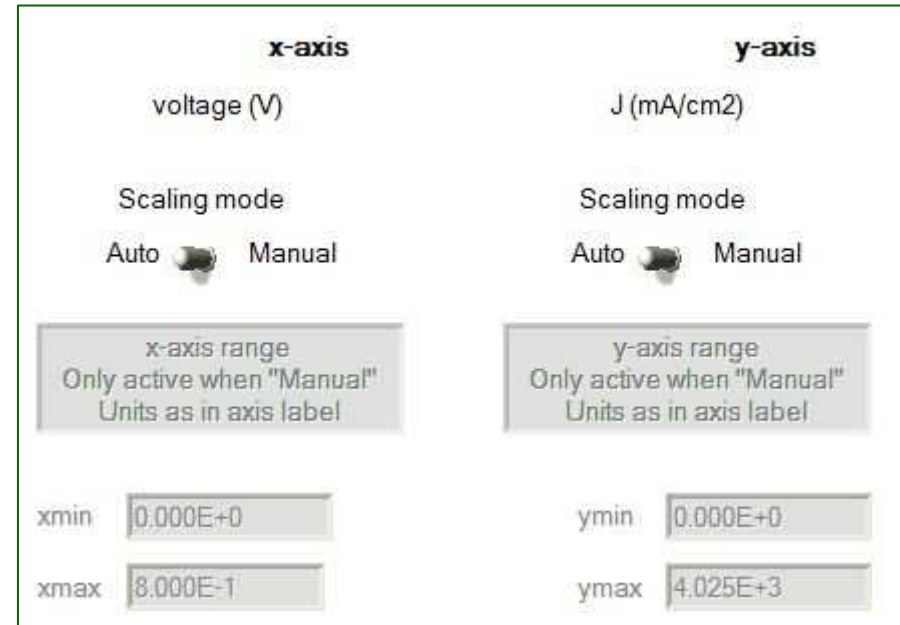
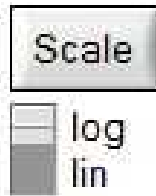


All grading data:



# Zooming and Scaling

- Set scaling on the scaling panel
- Switch between Linear & Logarithmic



- Press CTRL and draw a rectangle in a graph to zoom in
- Press CTRL and right mouse button to zoom out.



# The blue button

Other panels need input first!

- Allows browsing of the cell definition
- Makes sure you find minimized panels back
- Uneditable panels are dimmed

### Blue button Panel

Layer 1: p-CIGS  
Layer 2: n-CdS  
Graded Parameter

- eff. density of states  $NC(y)$
- electron mobility  $\mu_n(y)$
- opt. absorpt.  $\alpha(y, \lambda)$

Layer 3: n-ZnO  
New layer 4:  
Interface 2/3:

Only items in red can be edited immediately

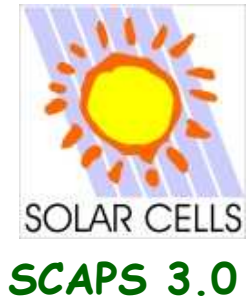
OK

exit all panels with OK    exit all panels with CANCEL

## EMERGENCY BUTTONS



- Press **F1** to get to cell definition panel (where you can access the blue button)
- Press **F2** to see the layer/interface panel



# Enjoy SCAPS



- SCAPS is freeware:
  - Register when using: ✉ Marc.Burgelman@Elis.Ugent.be  
Koen.Decock@Elis.Ugent.be
  - Cite when publishing:
    - M. Burgelman et al., *Thin Solid Films*, **361-362**, 527-532 (2000)
    - Other more specialized articles
- More Details:
  - Collection of (Add-on) user manuals
  - Contributions in literature

SCAPS info



SCAPS 3.0



# More Questions?

- Raise your hand and ask!
-  Marc.Burgelman@Elis.Ugent.be  
Koen.Decock@Elis.Ugent.be



- ☞ Please explain your problem, what you did and what you expected!
- ☞ Please add .def- or .scaps- file with sufficient comments & results.