Modeling Single- and Poly-crystal Silicon Solar Cells

CROSSLIGHT
Software Inc.

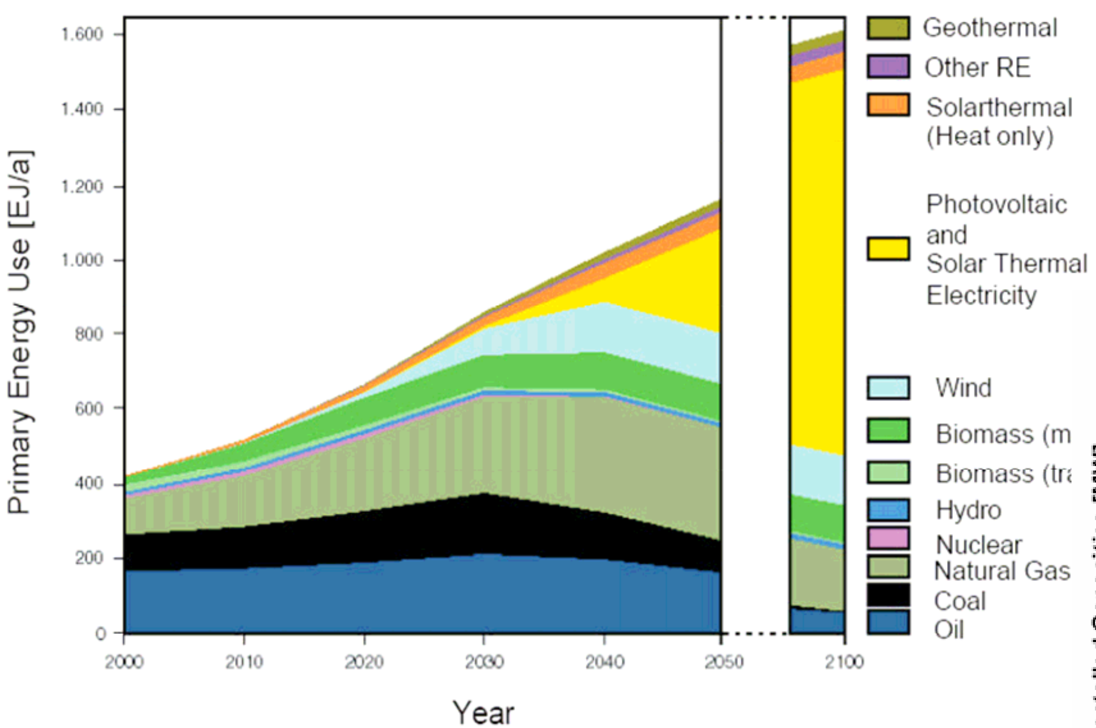
www.crosslight.com

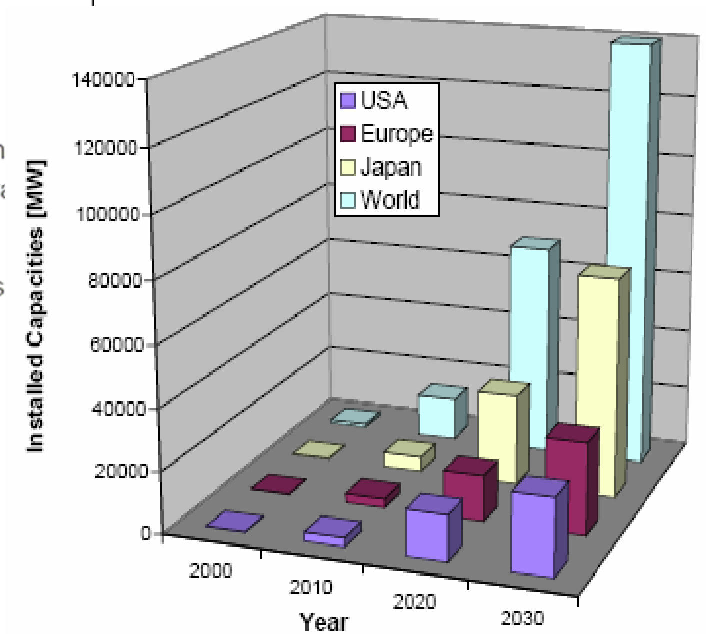
Contents

- **Introduction**
- Process simulation using CSuprem
- Theories and basic cell properties
- Si rear-contacted cells (RCC)
- Si PERT cells
- Summary

Hot market

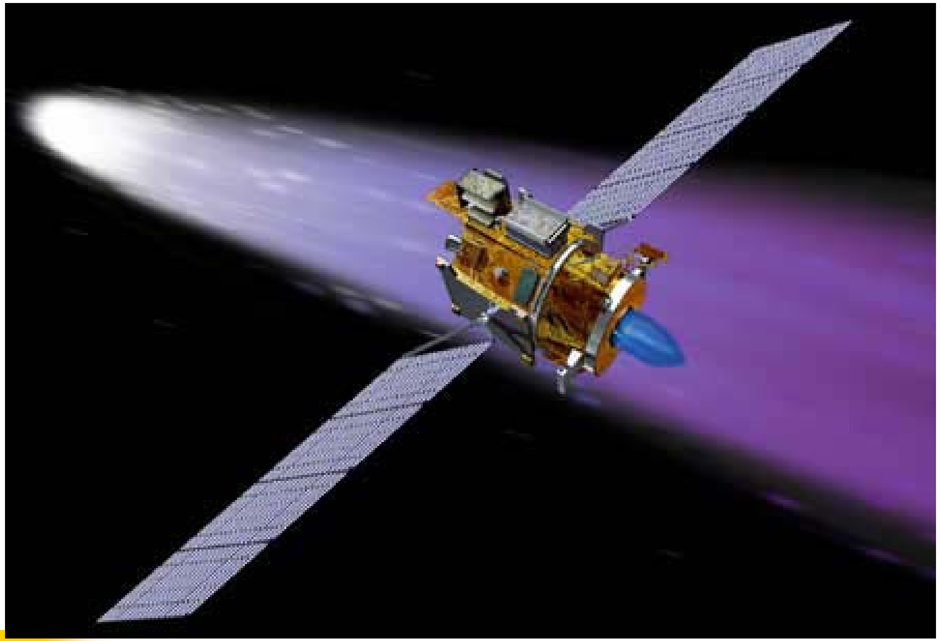
- **Increasing growth of global-wide market for photovoltaic system**





Efficient & affordable

- **Silicon solar cells - first demonstrated photovoltaic devices.**
- **Compatible with well-established fabrication technology.**
- **High efficiency & output at an affordable cost.**



source www.nrel.gov

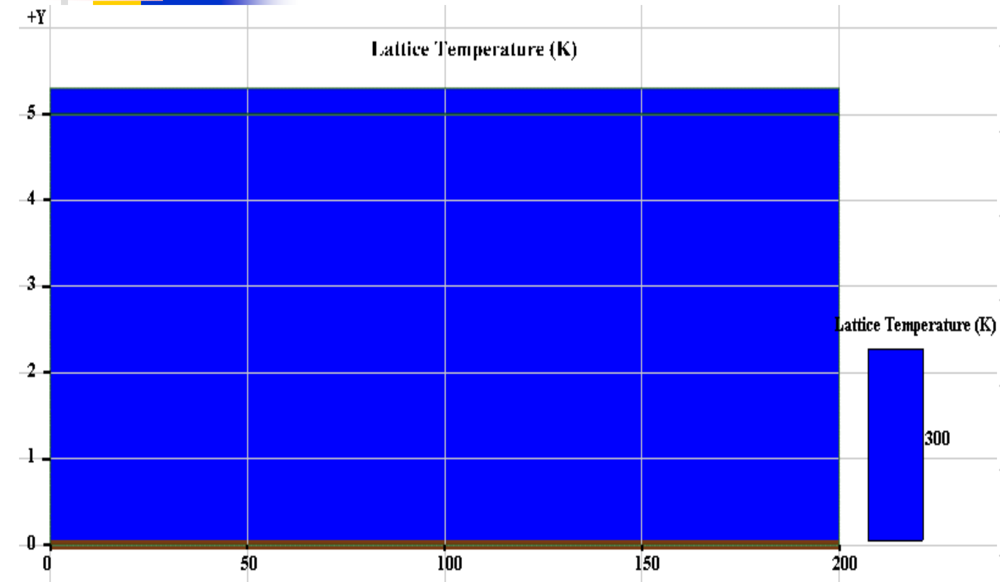
Process simulation: laser scribing or laser-fired-contact

- **Simulation challenges:**
  - Laser heating spot undergoes melting / phase transition.
  - A challenge to calculate heating temperature
  - Due to strong focusing of the laser beam, full 3D simulation for both process and device is preferred.

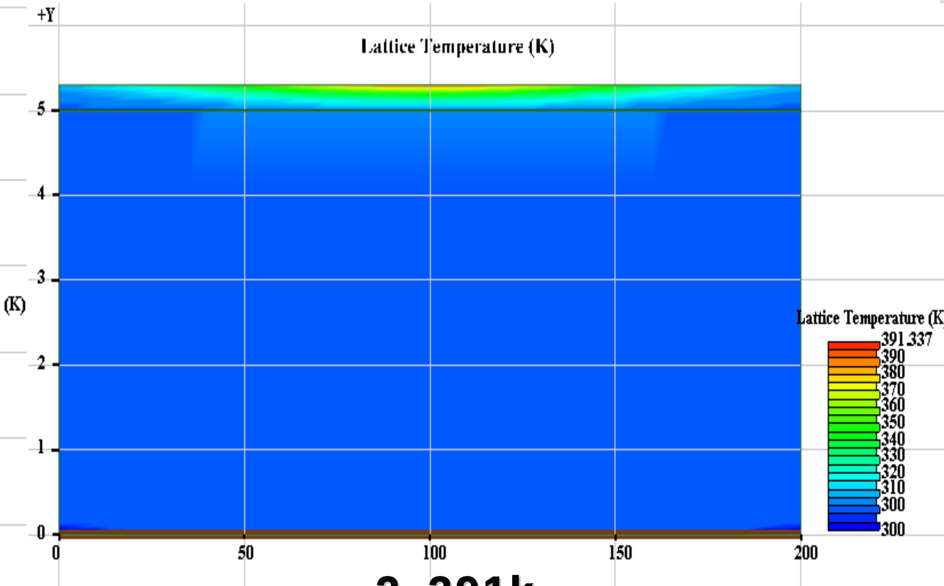
Simulation of laser scribing/laser-fired-contacts

- Use Csuprem (2D/3D) to set up mesh structure of tandem/ thin film layers.
- Transfer mesh data from Csuprem to APSYS to simulate local heating temperature profile based on laser parameters (pulse power, spot size, etc.).
- Transfer local heating temperature profile data from APSYS to Csuprem to simulate diffusion of aluminum impurity into silicon.
- Transfer mesh + doping profile data from Csuprem to APSYS to simulate solar-cell performance (I-V curves) under AM1.5.

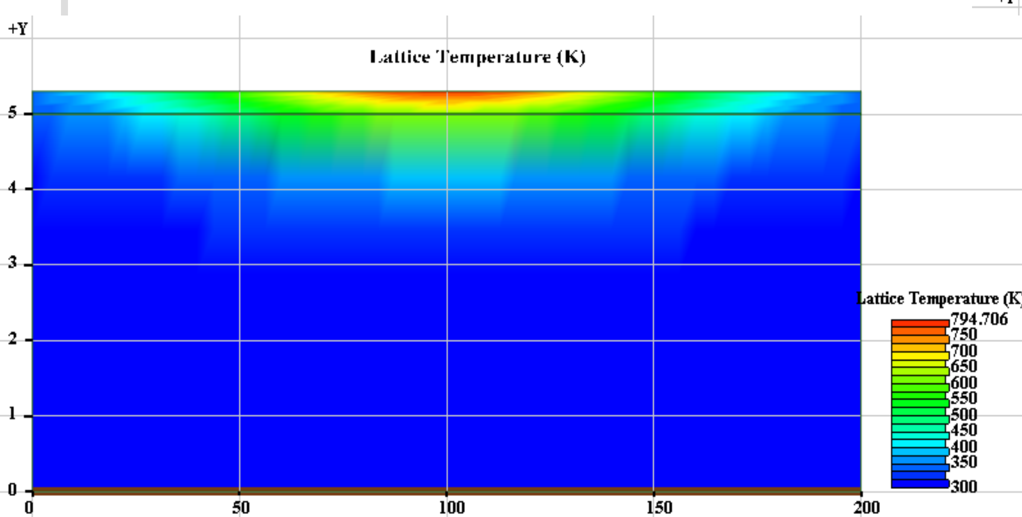
APSYS simulation of local heating profile



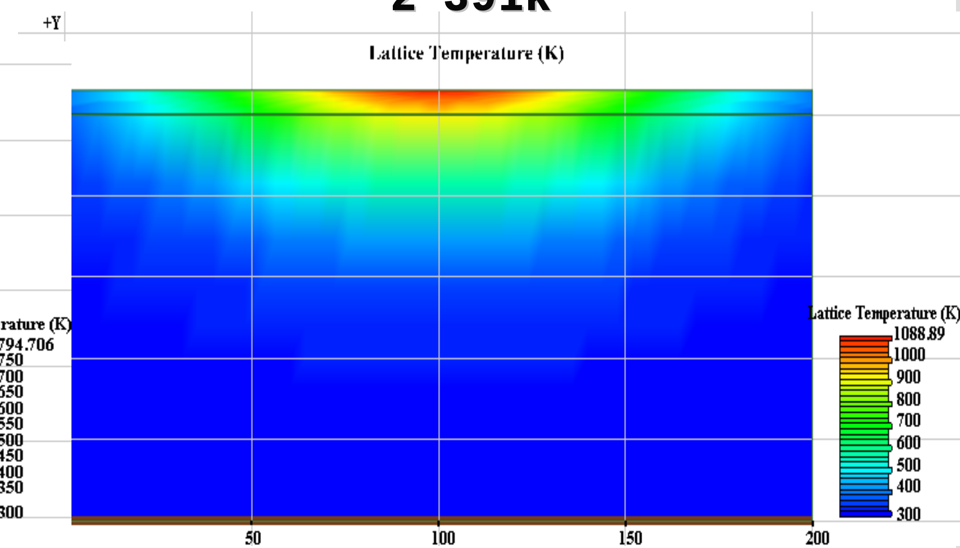
1 300k



2 391k



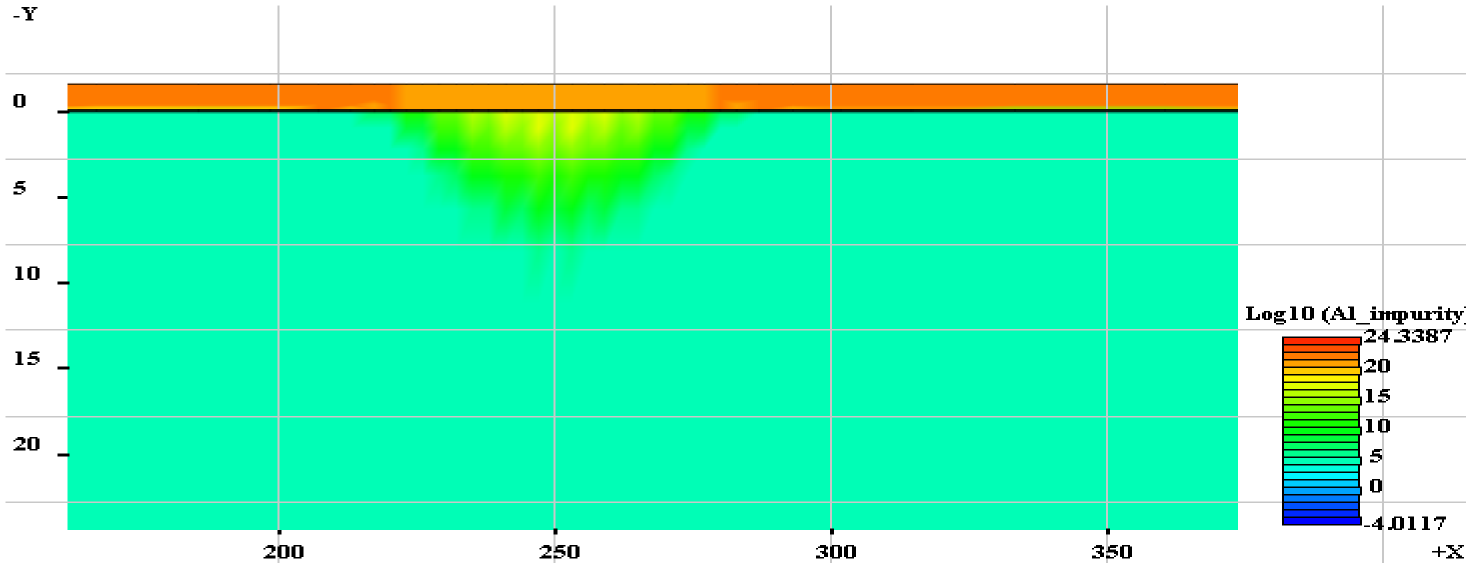
3 794k



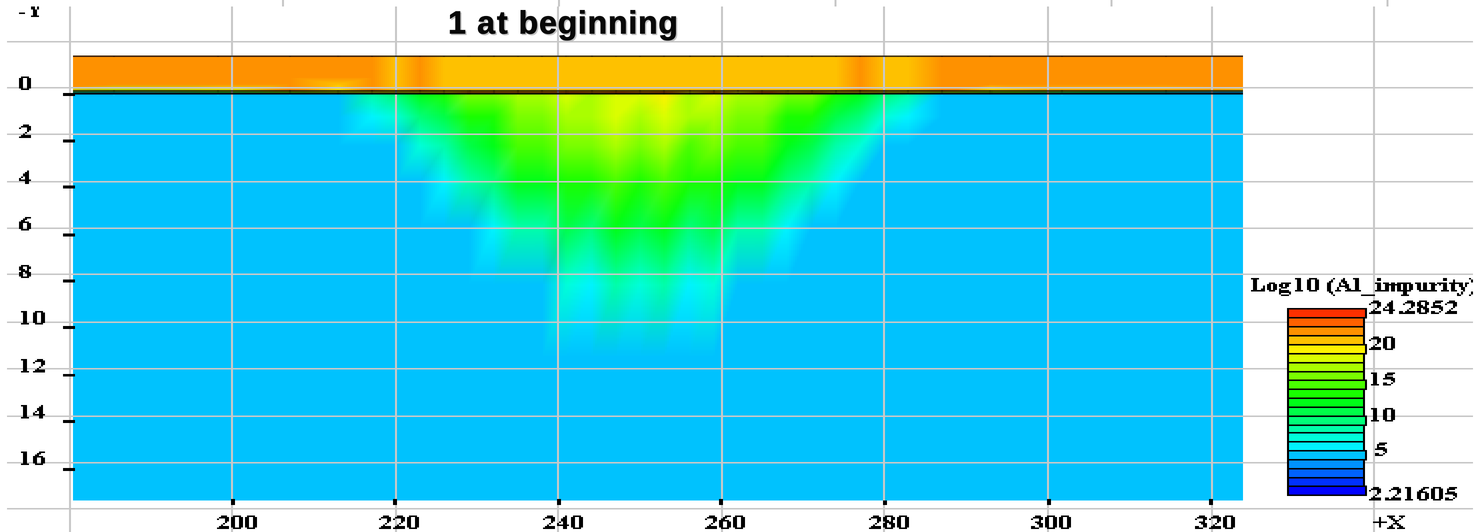
4 1089k

laser-induced temperature increase

CSuprem simulation of dopant diffusion



1 at beginning



2 several seconds after

diffusion of aluminum impurity in silicon substrate

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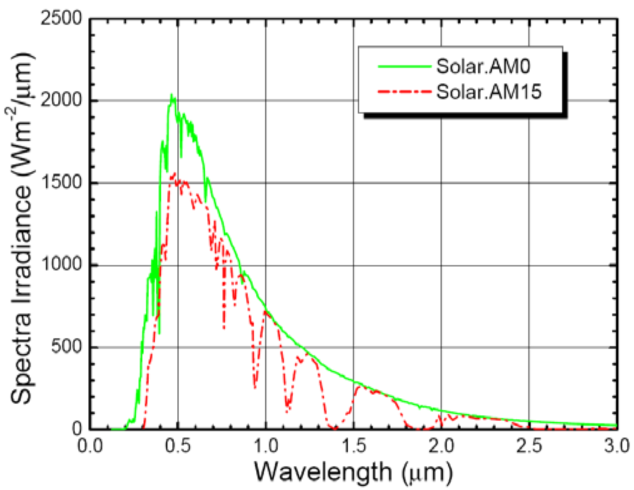
Theoretical background

- **Based on drift-diffusion theory, solving several coupled equations: Poisson, electron & hole drift-diffusion, etc…**



$$-\nabla\cdot\left(\frac{\varepsilon_0\varepsilon_{dc}}{q}\nabla V\right) = -n+p+N_D(1-f_D)-N_Af_A+\sum_j N_{tj}\left(\delta_j - f_{tj}\right)$$

$$\nabla\cdot J_n - \sum_j R_n^{tj} - R_{sp} - R_{st} - R_{au} + G_{opt}(t) = \frac{\partial n}{\partial t} + N_D\frac{\partial f_D}{\partial t},$$

$$\nabla\cdot J_p + \sum_j R_p^{tj} + R_{sp} + R_{st} + R_{au} - G_{opt}(t) = -\frac{\partial p}{\partial t} + N_A\frac{\partial f_A}{\partial t}.$$

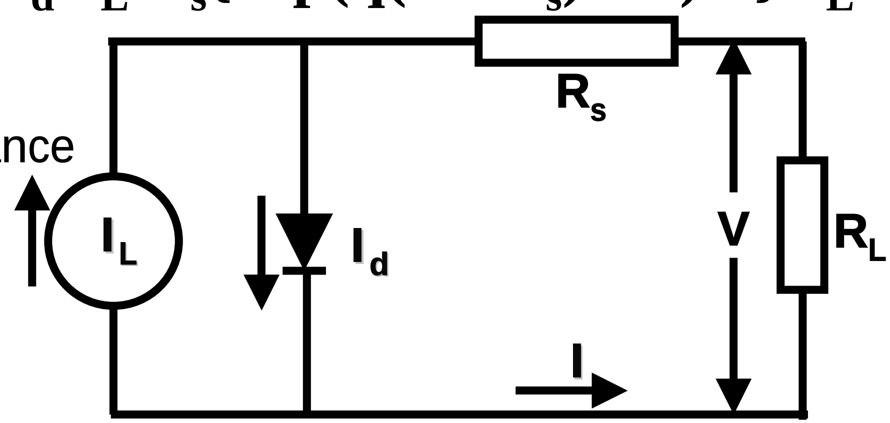
- **Solar spectrum**
- **Equiv. external circuit**

I_L: source current; R_L: load resistance

I_s: diode saturation current

R_s: cell series resistance due to defects and interfaces; Higher R_s, lower efficiency

$$I=I_d-I_L=I_s\{\exp(q(V-IR_s)/kT)-1\}-I_L$$

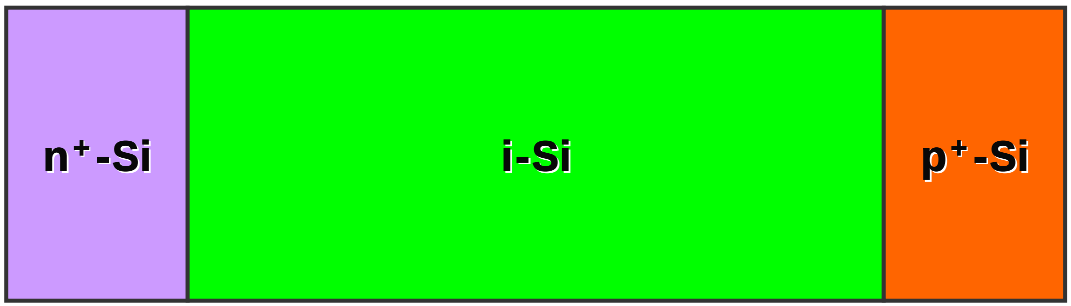


Advanced model features

- Bulk/surface recombination models.
- Bulk/surface trapping effects.
- Optical coating model (with multi-layer optical interference effects).
- 3D raytracing combined with multiple layer optical coating models. Raytracing performed over the full solar spectrum.
- Wavelength dependence effects in solar spectrum, bulk material and optical coating.

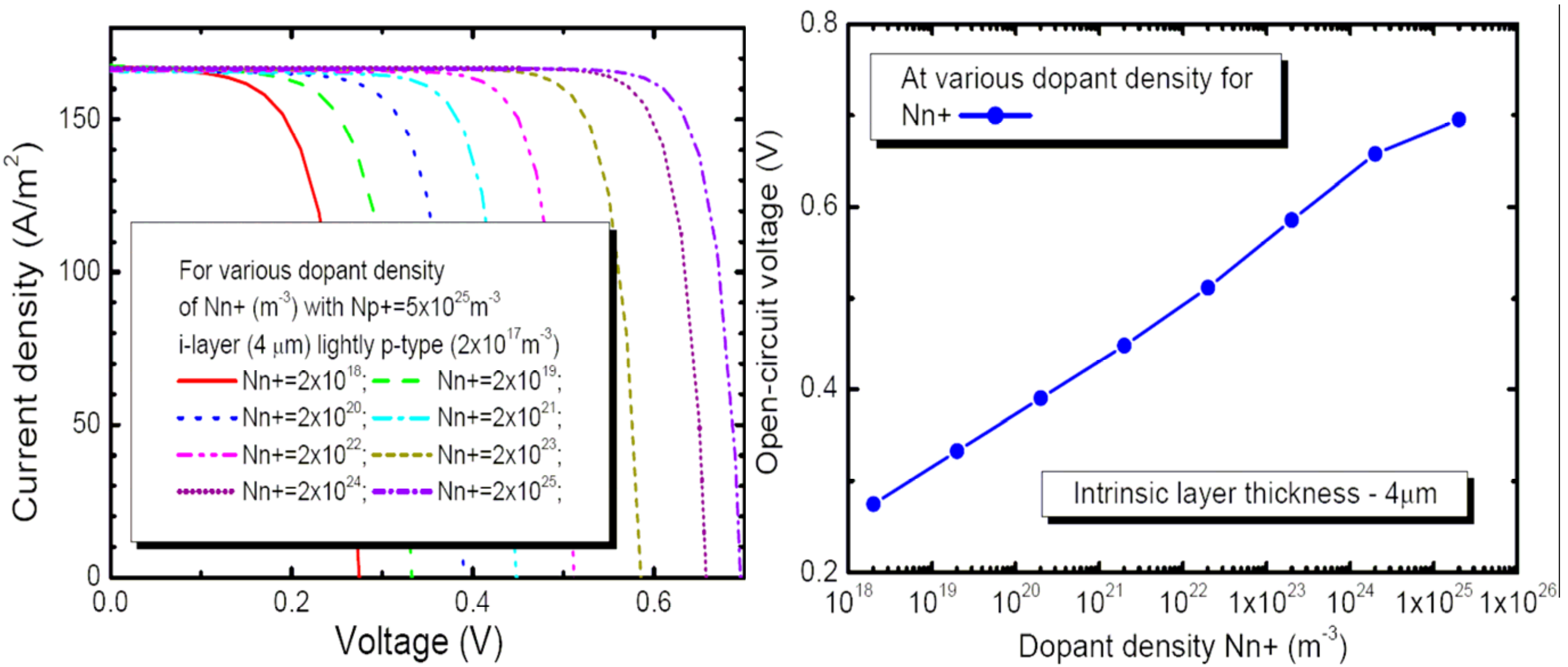
Si-PIN solar cells

- **Electron & hole mobility & lifetime models calibrated with experimental data.**
- **Silicon-PIN diode thin film solar cell simulated.**



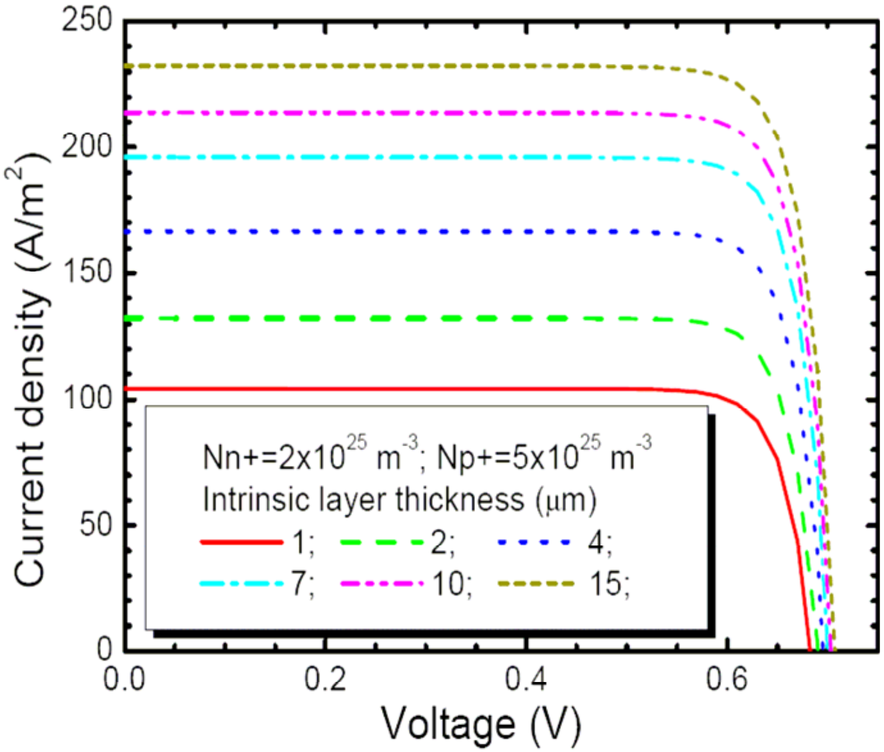
- **Varying n^+ layer dopant density while keeping others unchanged.**
- **Varying i-layer thickness while keeping others unchanged.**
- **Temperature, surface recombination effect & coating effects**

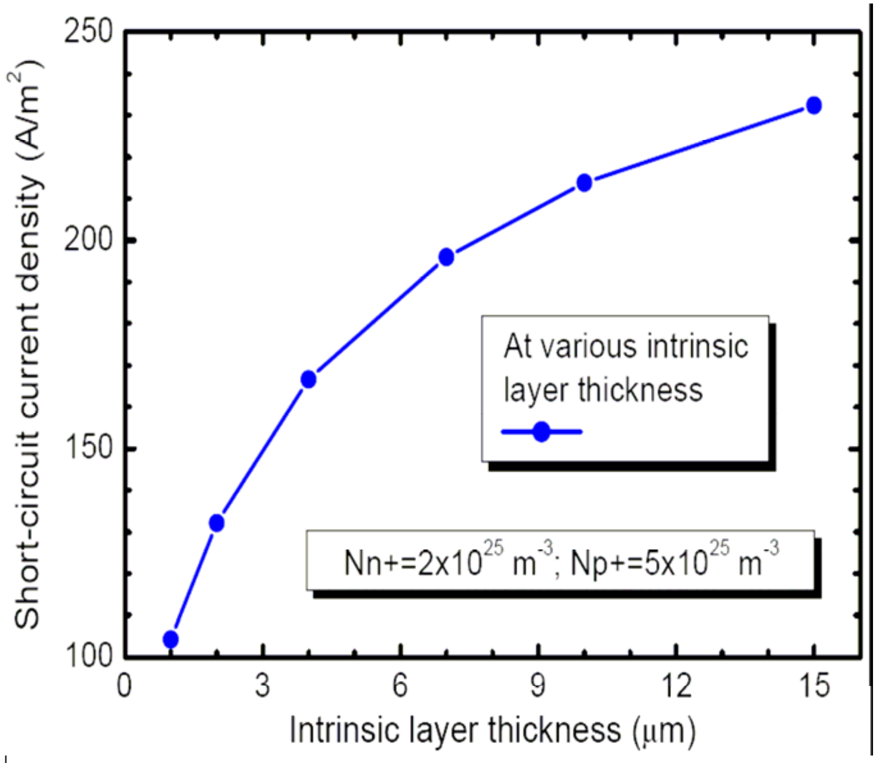
Si-PIN doping effects: I-V Curve & Voc



- **Voc enhancement caused by reduced diode saturation current Is (enhanced built-in voltage) with increased n^+ dopant density (see "Physics of Semiconductor Devices", S. M. Sze).**

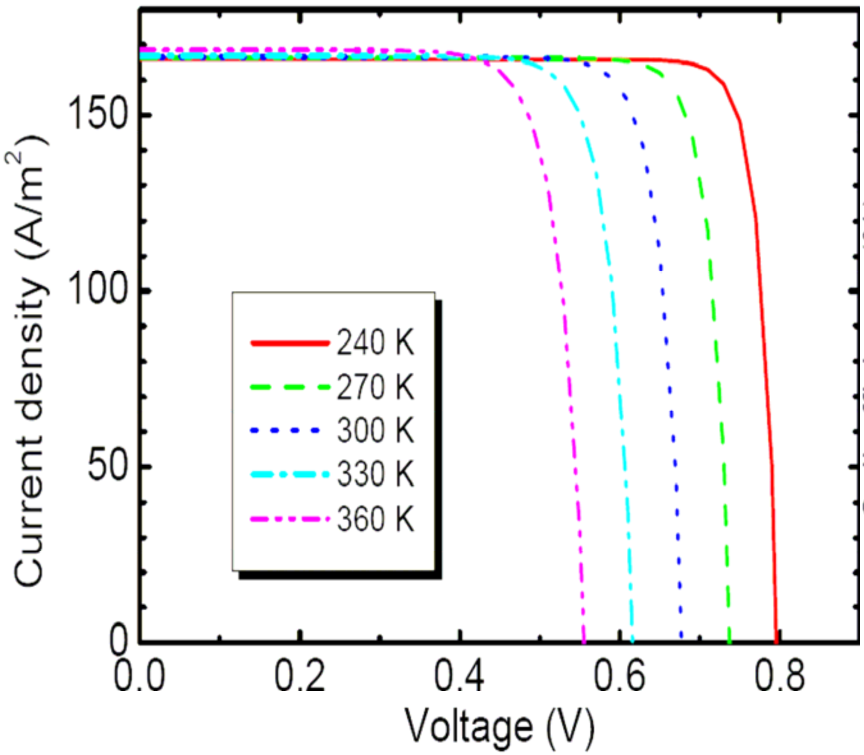
Si-PIN layer thickness effects: I-V curve & Isc

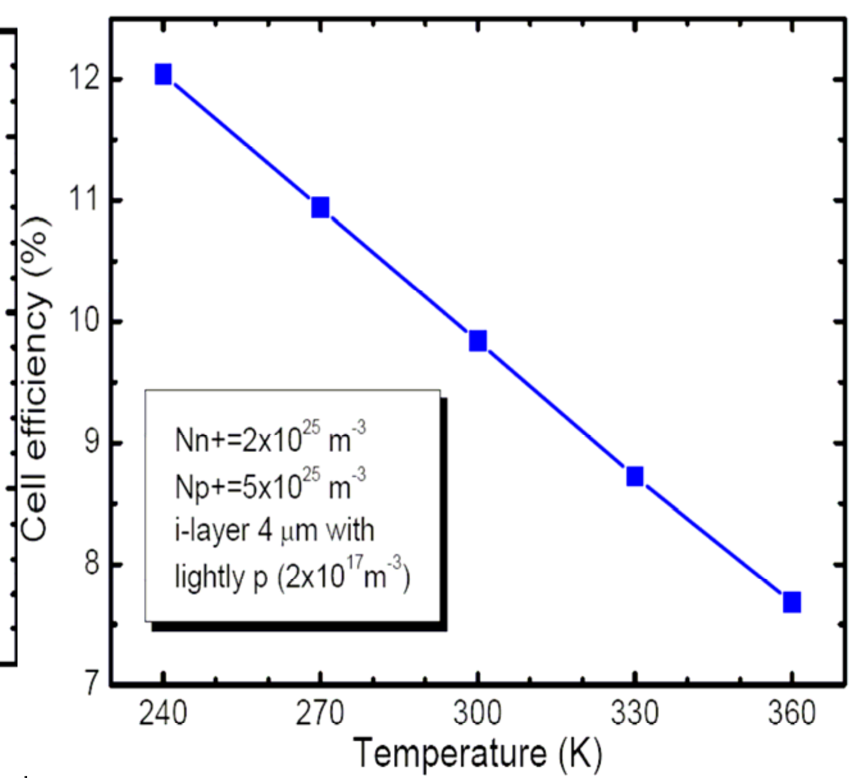




- **Short-circuit current enhanced due to the enhancement of photo-generated carriers with wide intrinsic absorption layer.**

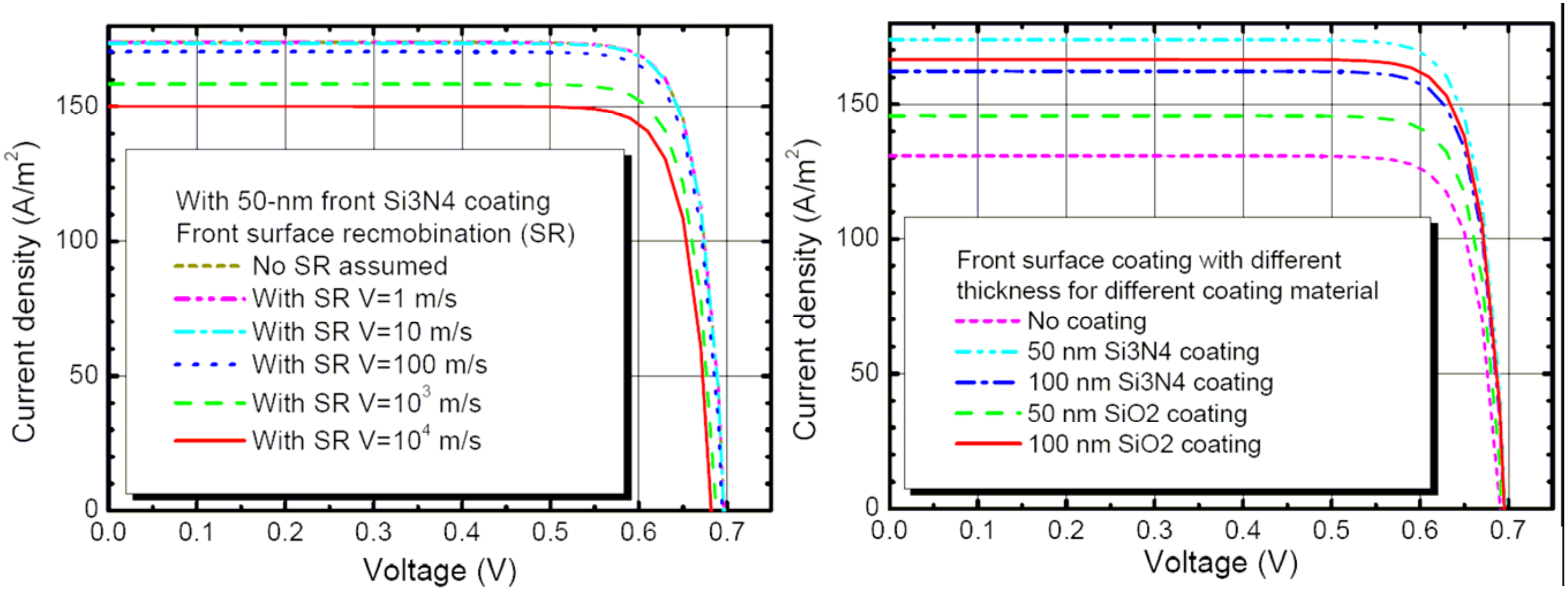
Si-PIN temperature dependence





- **Cell performances degrades as temperatures increases, consistent with semiconductor diode & cell theory & some observed exper. results [Refs: MA Green, Prog. Photovolt: Res. Appl., 11 (2003) pp333-340, & DL Pulfrey, Photovoltaic Power Generation, Van Nostrand Reinhold, New York 1978].**

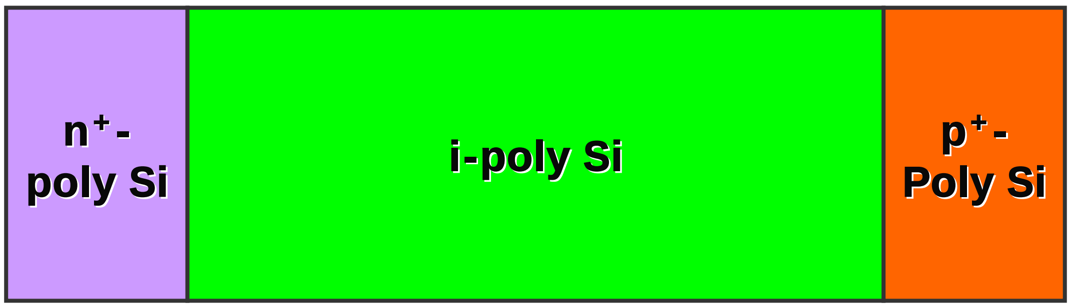
Si PIN surface recombination & coating effect



- **I-V curves with various front surface recombination velocity. Back surface recombination (BSR) effect negligible for small BSR velocity.**
- **There is optimal coating layer thickness for specific coating material.**

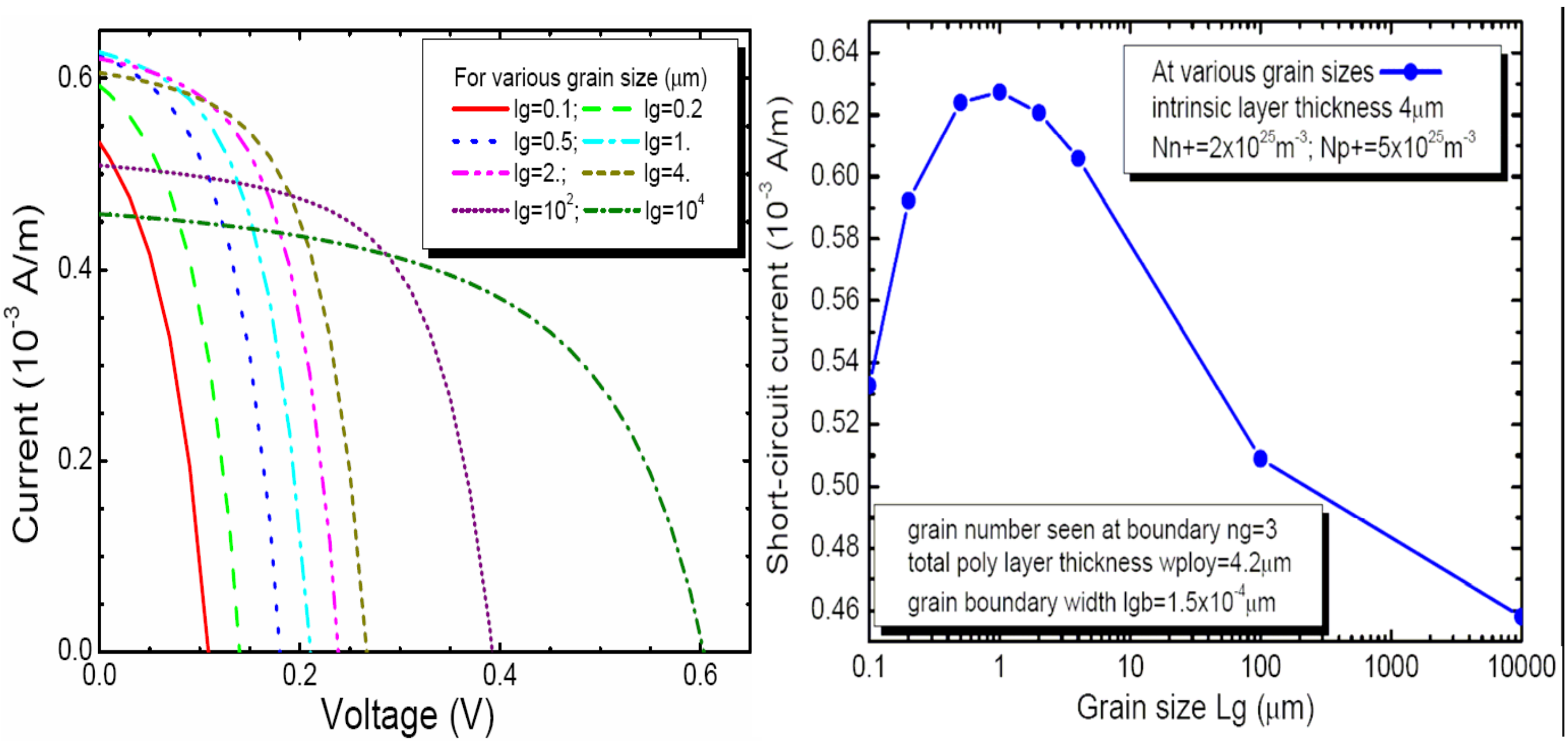
Poly-Si PIN solar cells

- **Electr. & hole mobility & lifetime models same as Si inside grain.**
- **Grain boundary influence on mobility & lifetime implemented.**



- **Poly Si PIN diode solar cell simulated to investigate grain size effect on the cell performance.**
- **Varying grain size while keeping other parameters unchanged.**

Poly-Si grain size effects: I-V curve & Isc



- **Grain size affects both short circuit current & open circuit voltage.**

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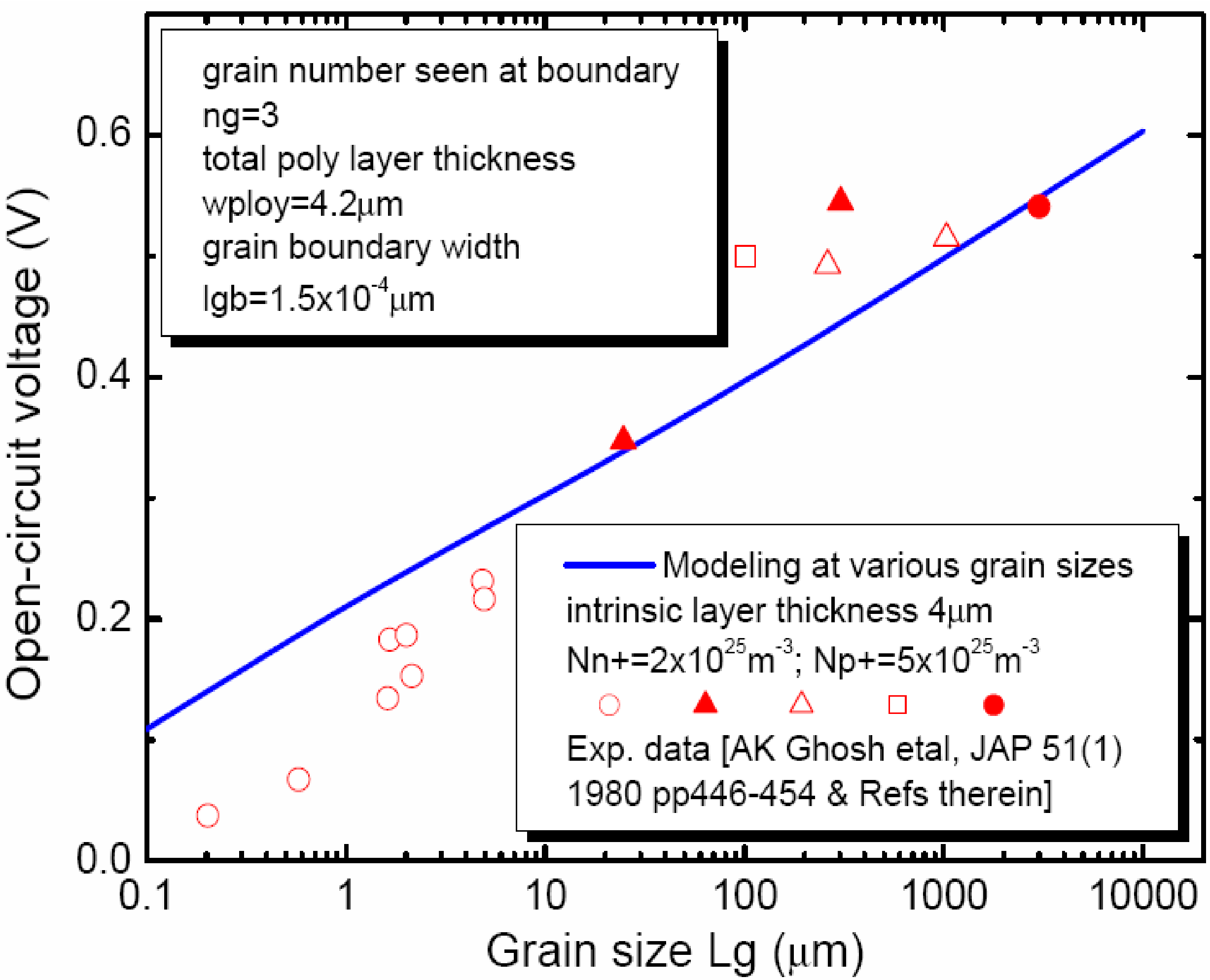
Poly-Si V_{oc} in comparison with experiment



- **Voc in agreement with experimental results.**

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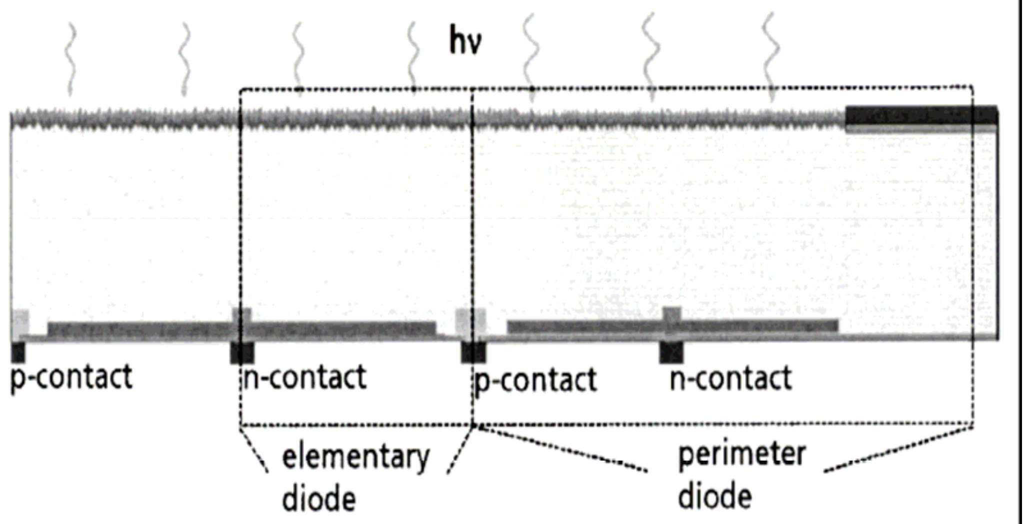
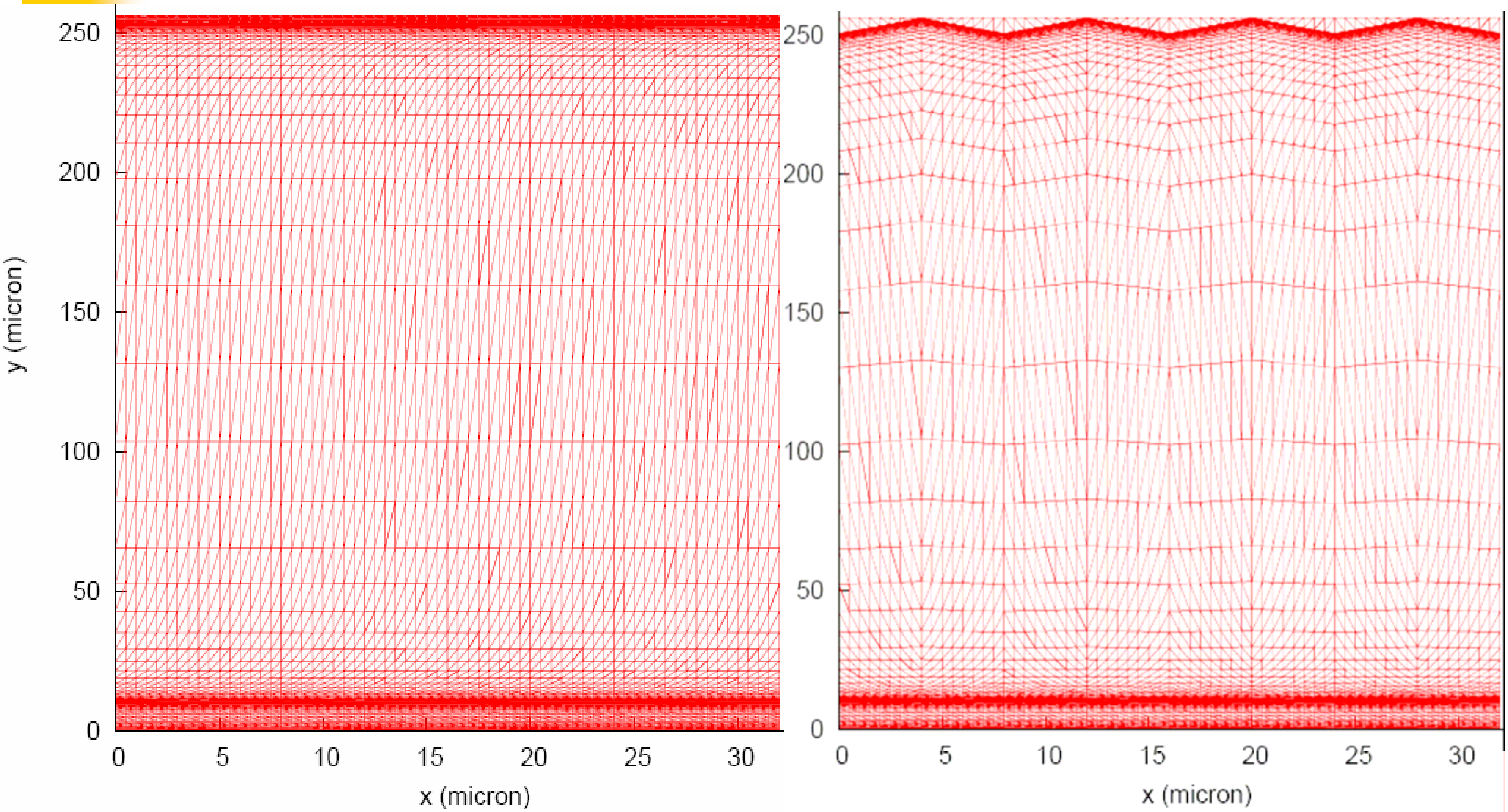
Rear-contacted cells RCC with front texture



J Dicker et al, JAP, V91N7, 2002, pp4335-4343

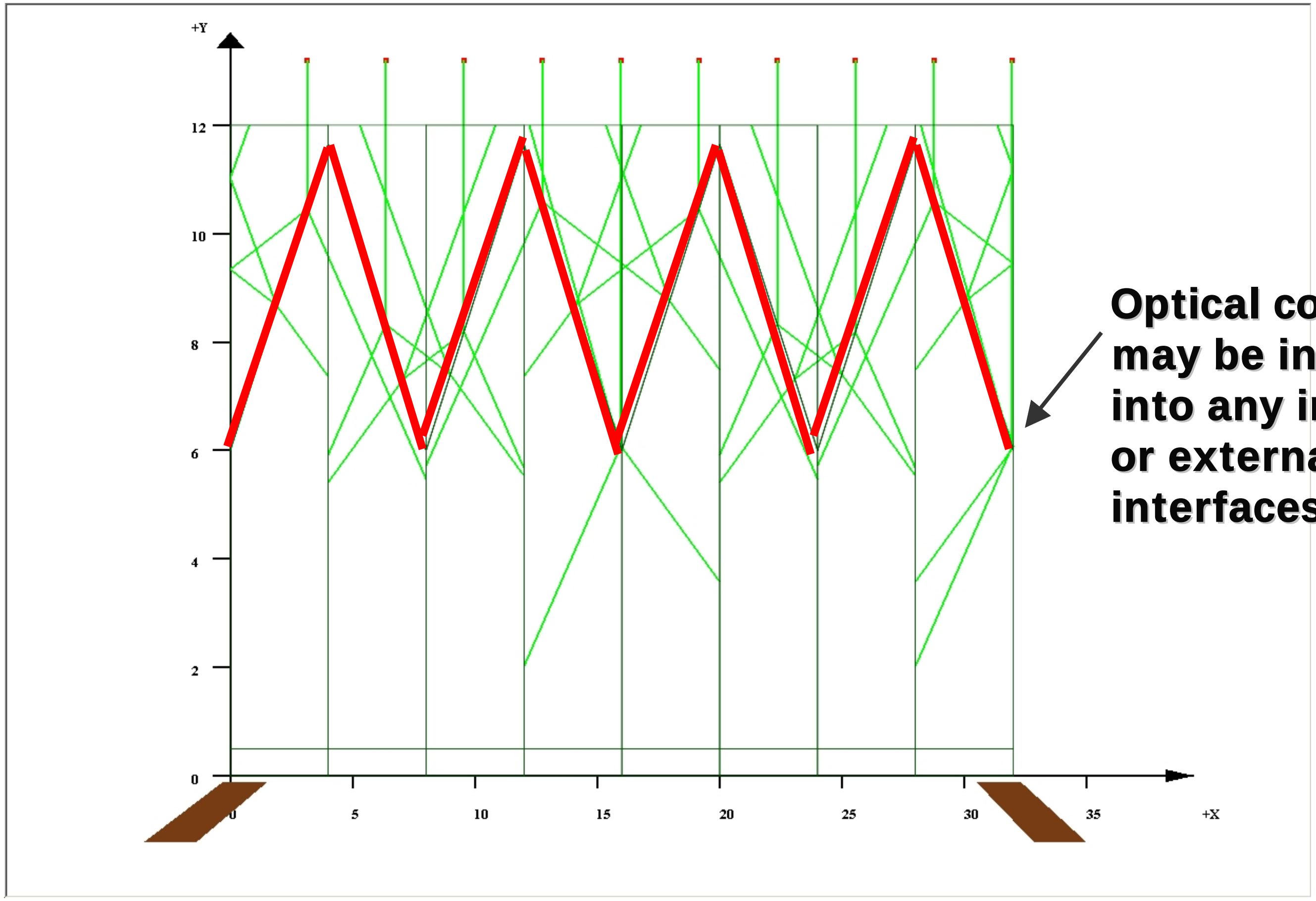
- **Setup of 2D device structure with Crosslight LayerBuilder.**
- **Setup of 2D triangle shape with Crosslight GeoBuilder.**
- **Enhanced optical absorption computed with ray-tracing technique. Comparing flat and triangle textured cases.**

RCC - Mesh comparison



- **Structure mesh: flat (left) & triangle (right). Structure not to the scale (all triangles at front with height 5.6494 μm & equal sides; 54.7 Deg between side & horizontal direction).**

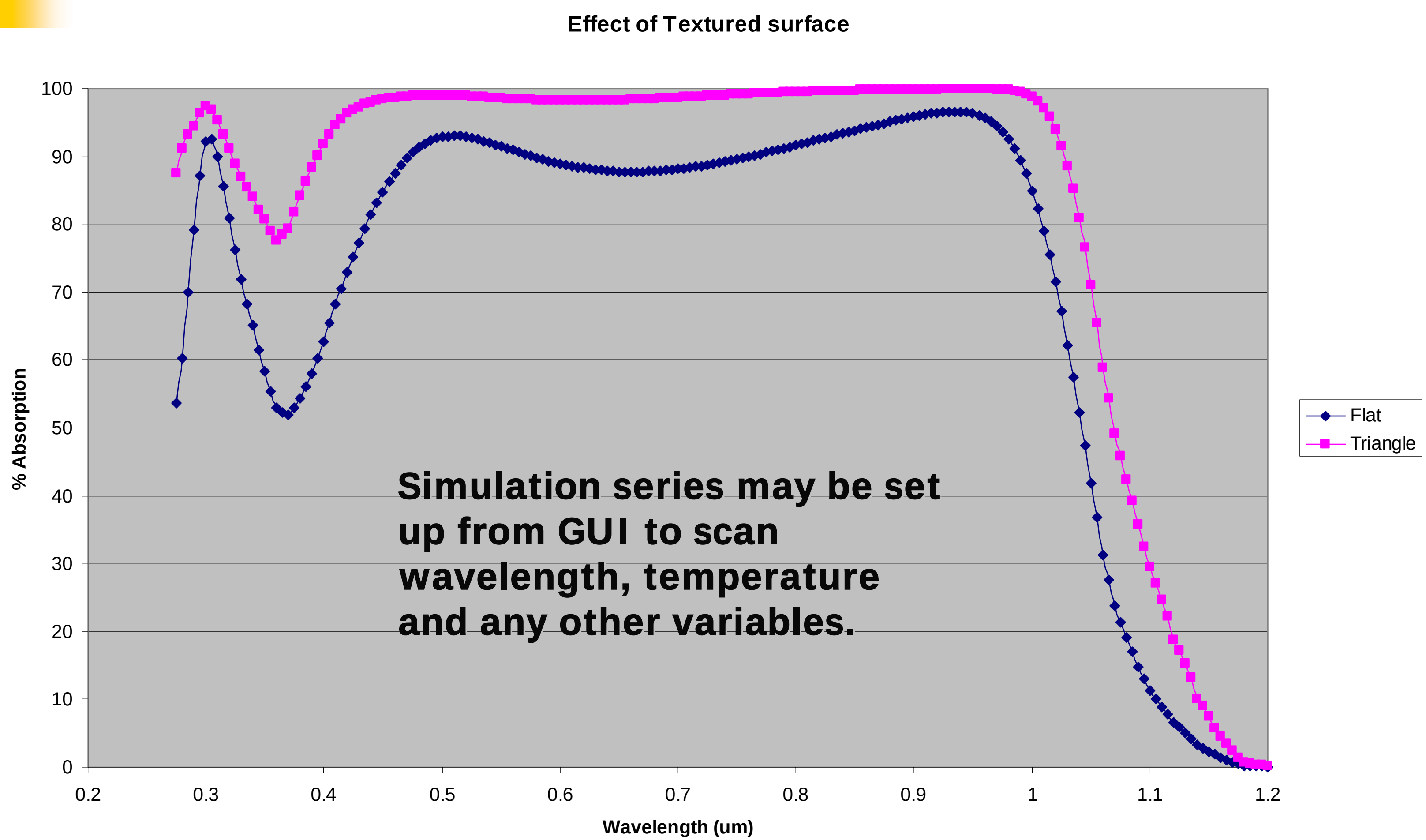
RCC – Ray tracing



Optical coating may be inserted into any internal or external interfaces

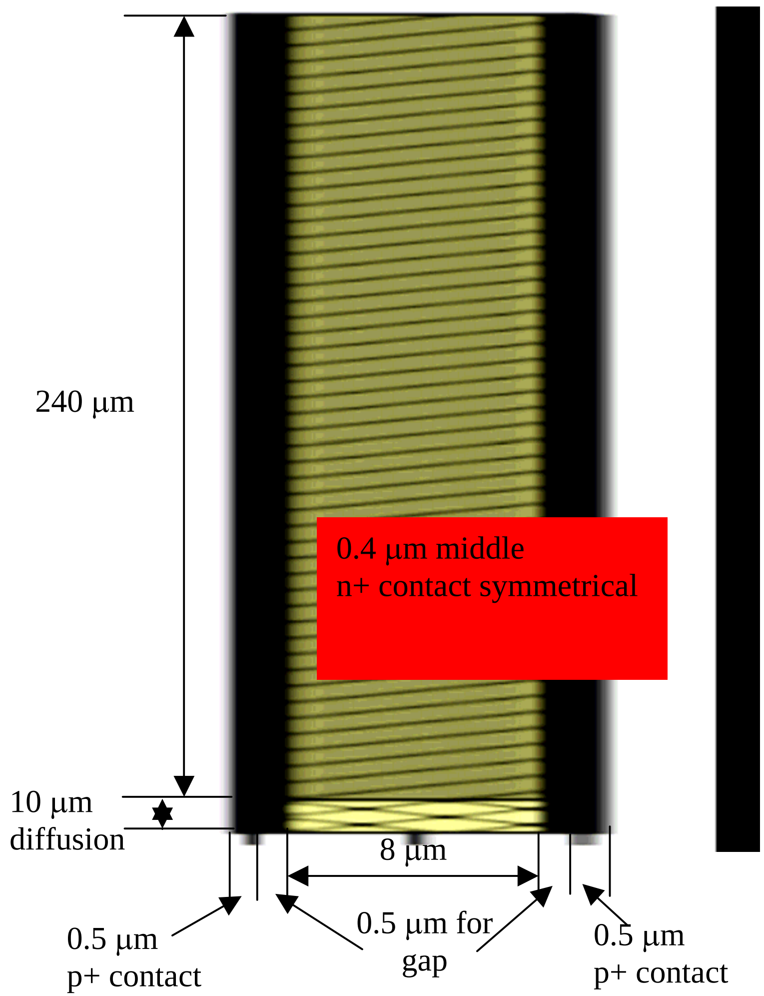
- Ray tracing shows how reflected incident rays have a chance to re-enter the device, thereby increasing light absorption. Device truncated for clarity.

RCC – Absorption enhancement

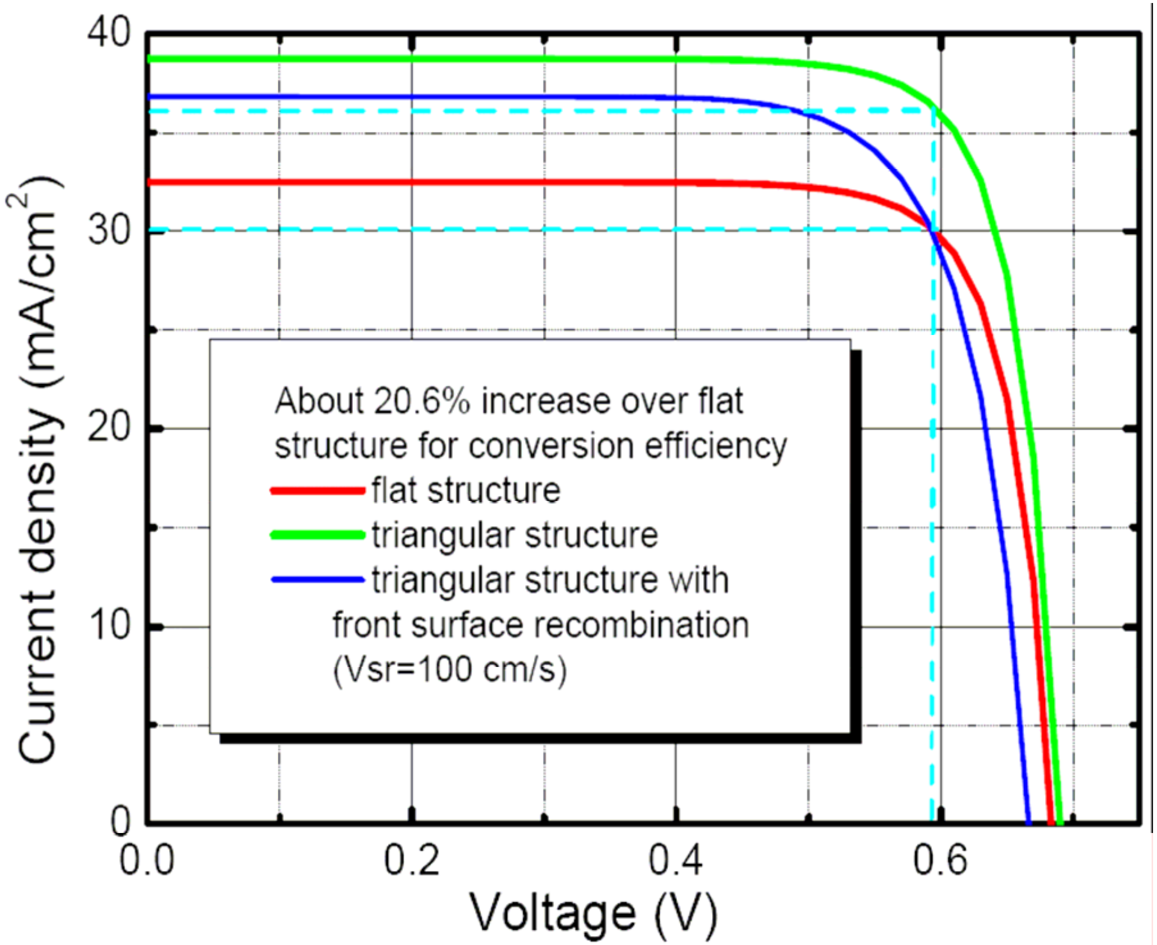


- **Ray tracing can also include the effects of multi-layer optical coatings: interference effects, wavelength-dependent refractive index, etc ….**

Incorporating scale factor – narrow device

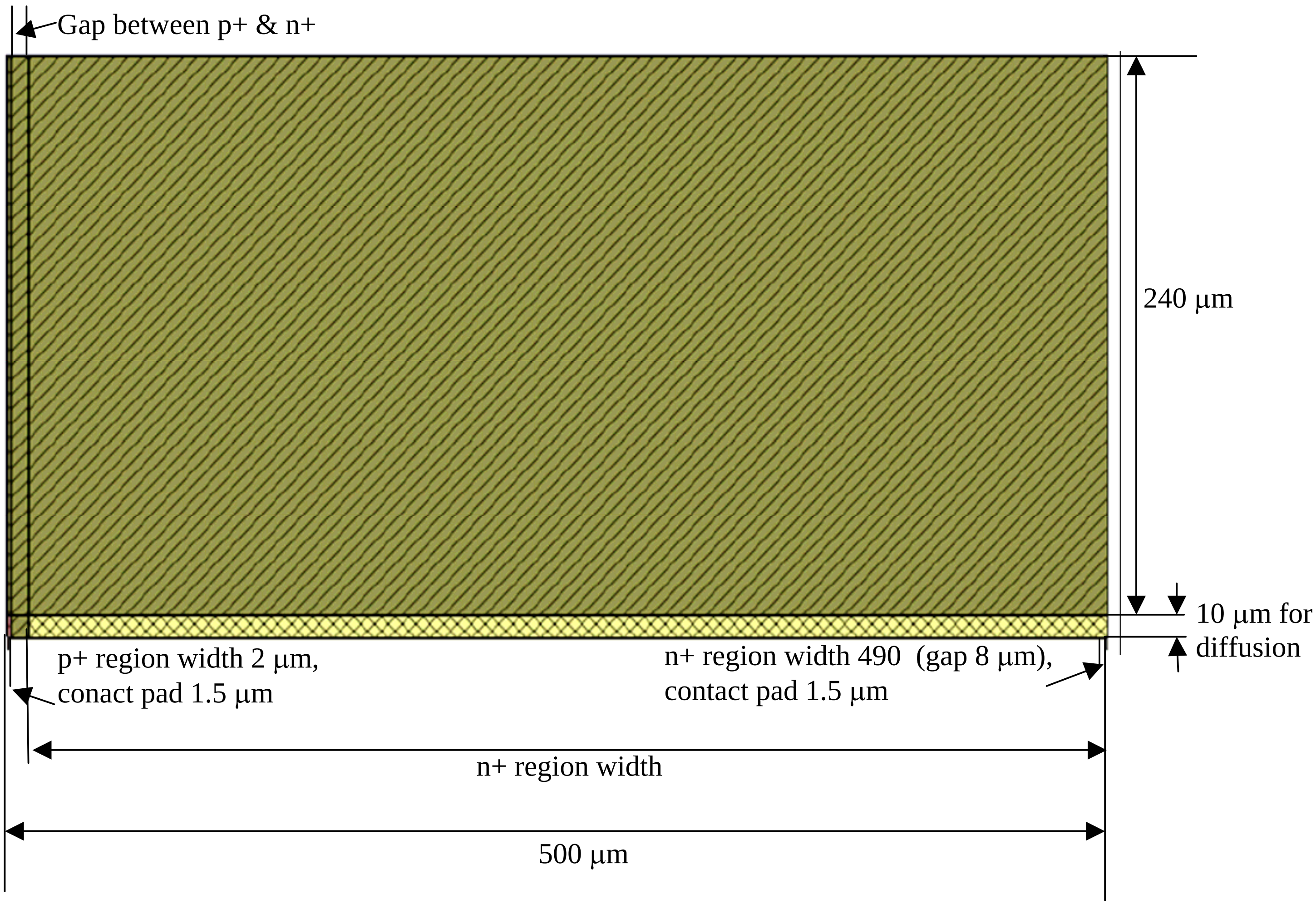


RCC narrow device – I-V curve comparison



- **Triangle structure leads to 20.6% increase over flat structure, indicating actual cell conversion efficiency could increase from 17.6% (assumed for flat) to 21.23% (triangle textured).**

Incorporating scale factor – large device



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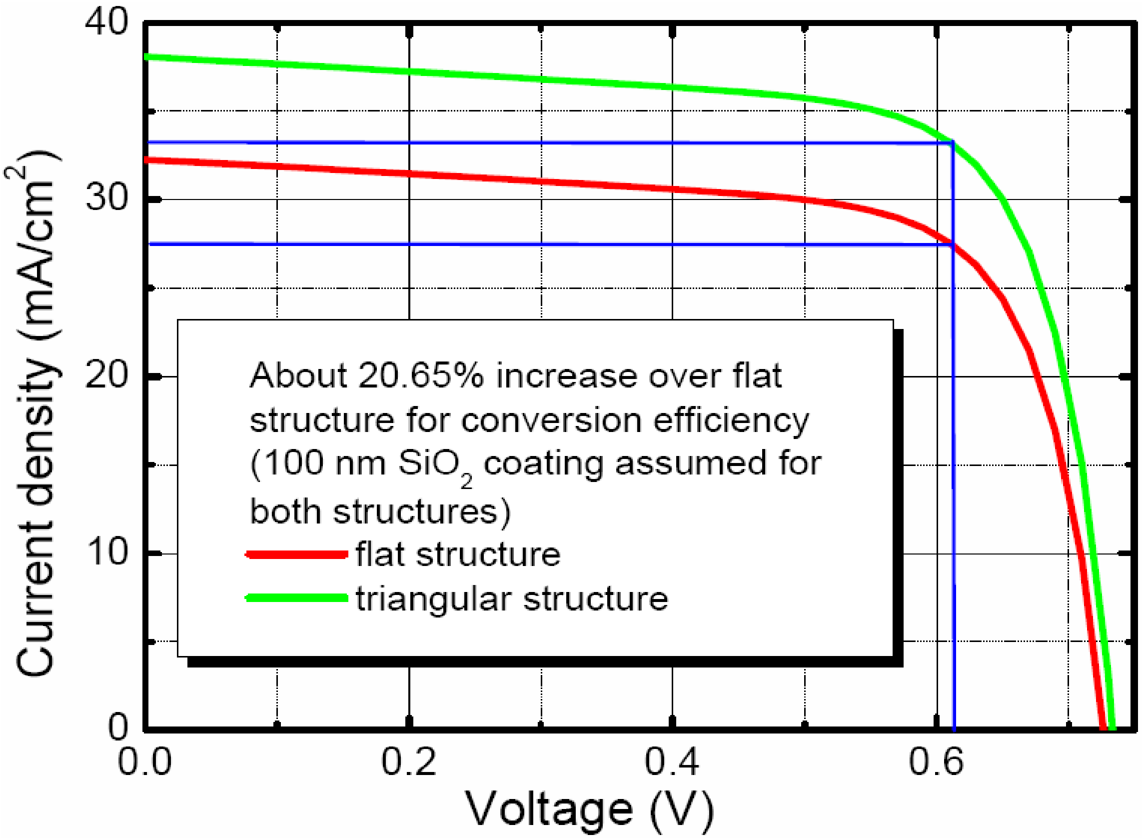
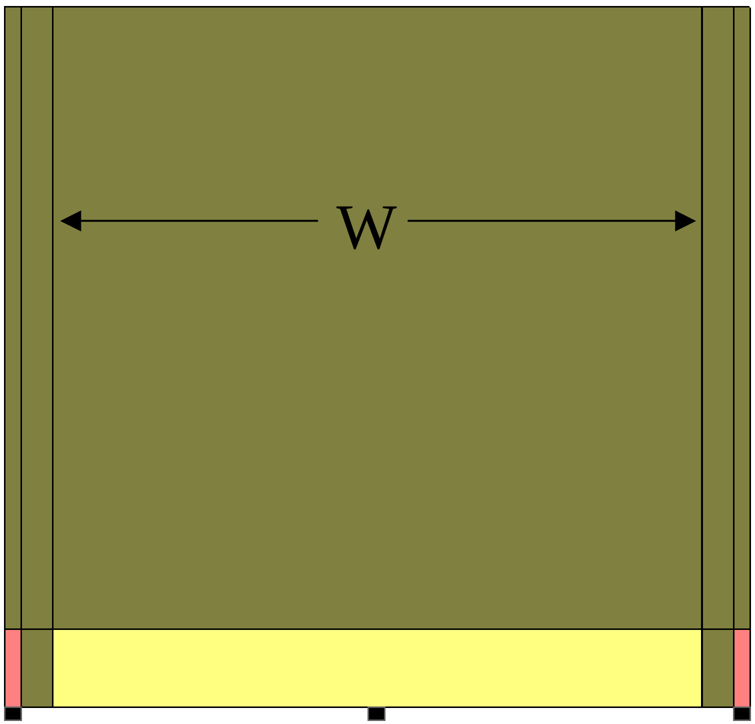
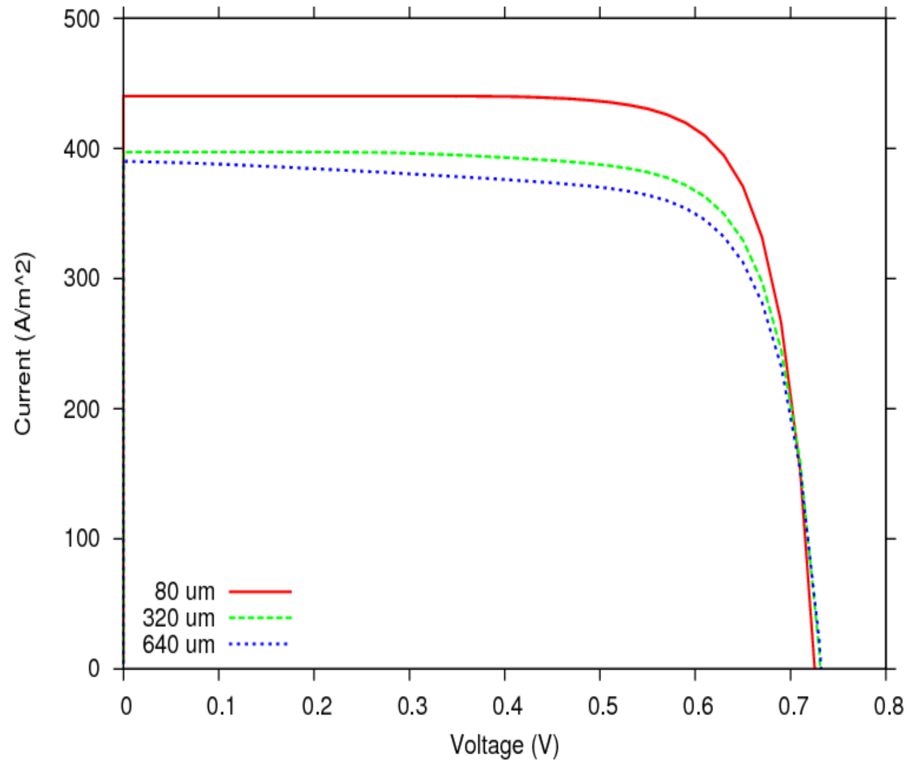
RCC large device – I-V curve comparison



- **Triangle structure leads to 20.65% increase over flat structure, indicating actual cell conversion efficiency could increase from 17.6% (assumed for flat) to 21.23% (triangle textured). Resistive slope at the ceiling is due to the enlarged series resistance with large separation between p & n contact pads.**

Effect of series resistance

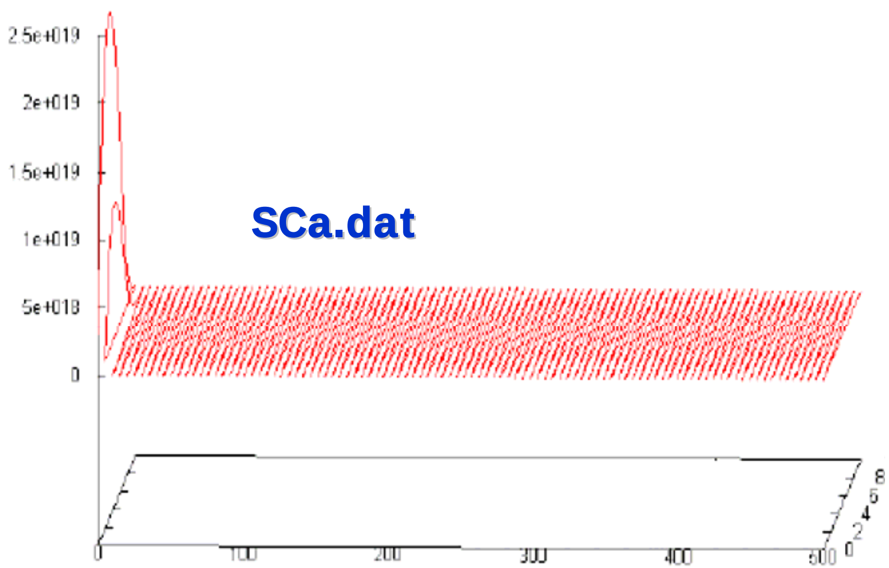


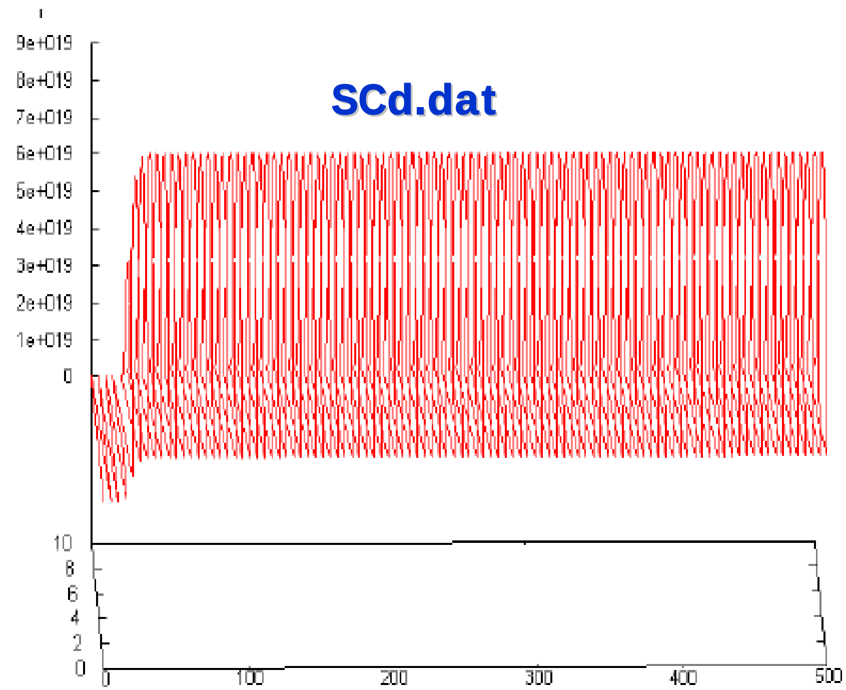


- **With various width; Larger W, higher R_s, lower efficiency.**

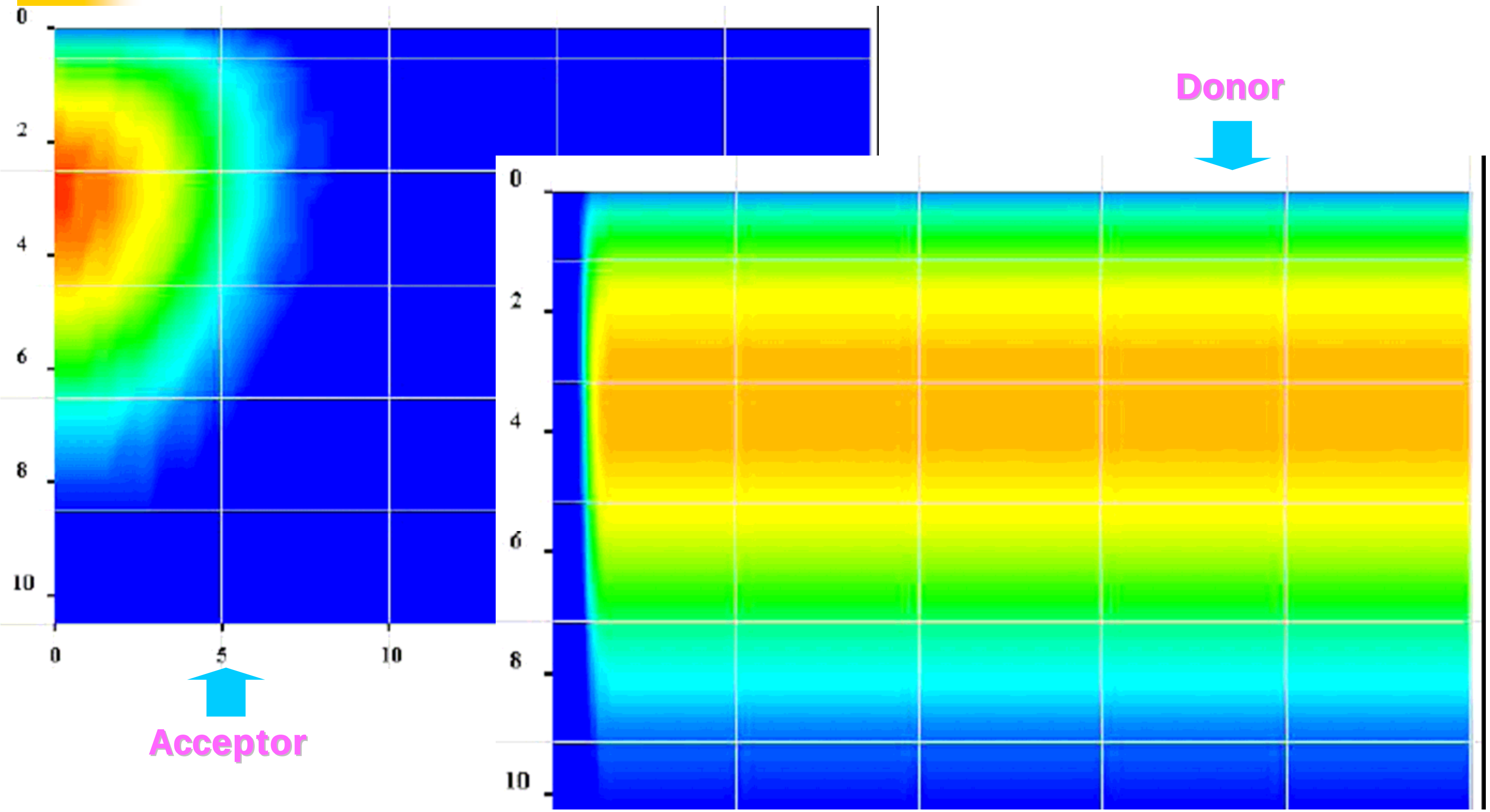
Importing doping profile from CSuprem

- **Use CSuprem (another package) to generate diffSC.str file.**
- **Use attached show2d.exe to generate acceptor & donor doping profile data diles, SCa.dat & SCd.dat.**
- **Use "doping ..." command lines in sol file to import these doping profiles.**



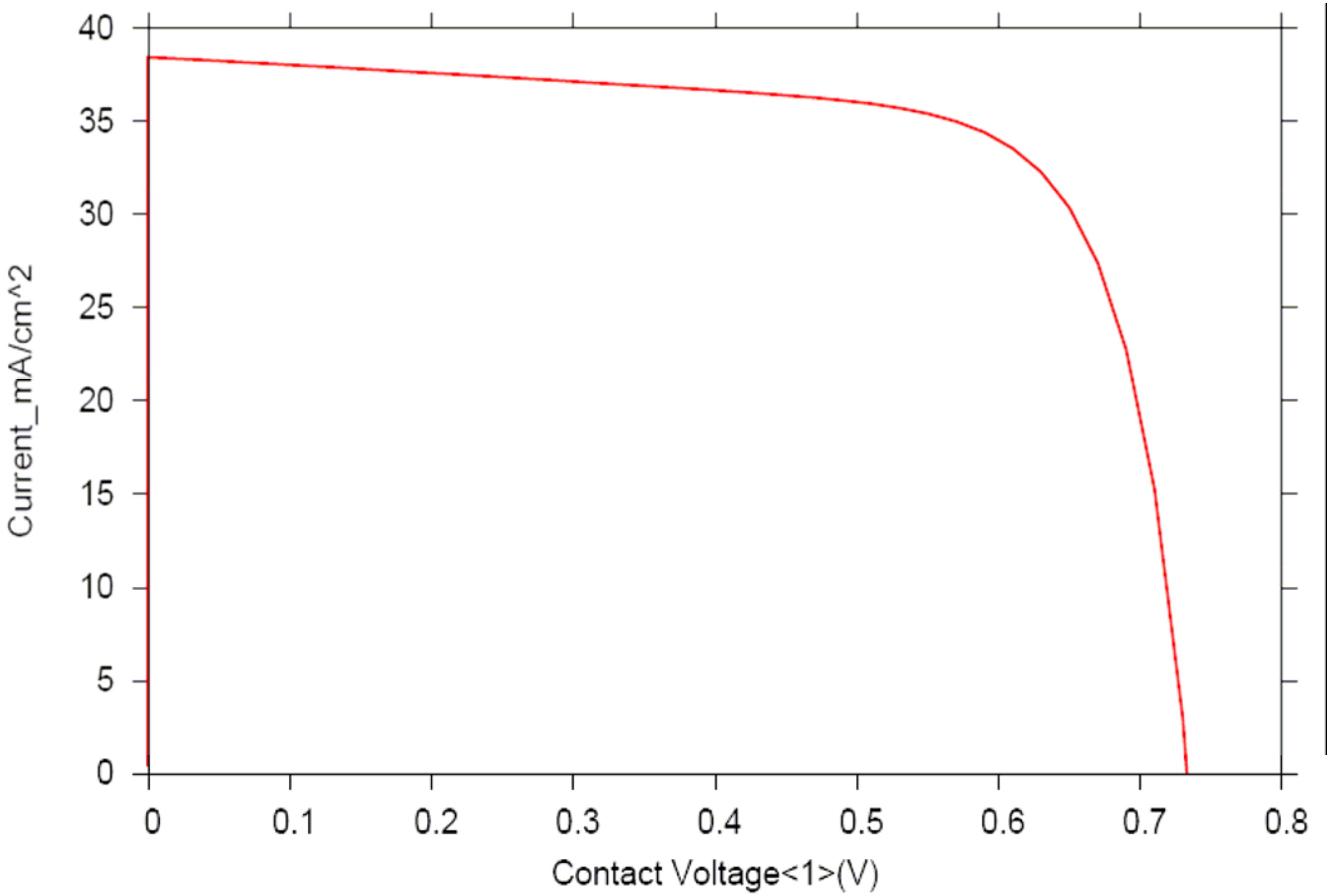


CSuprem output



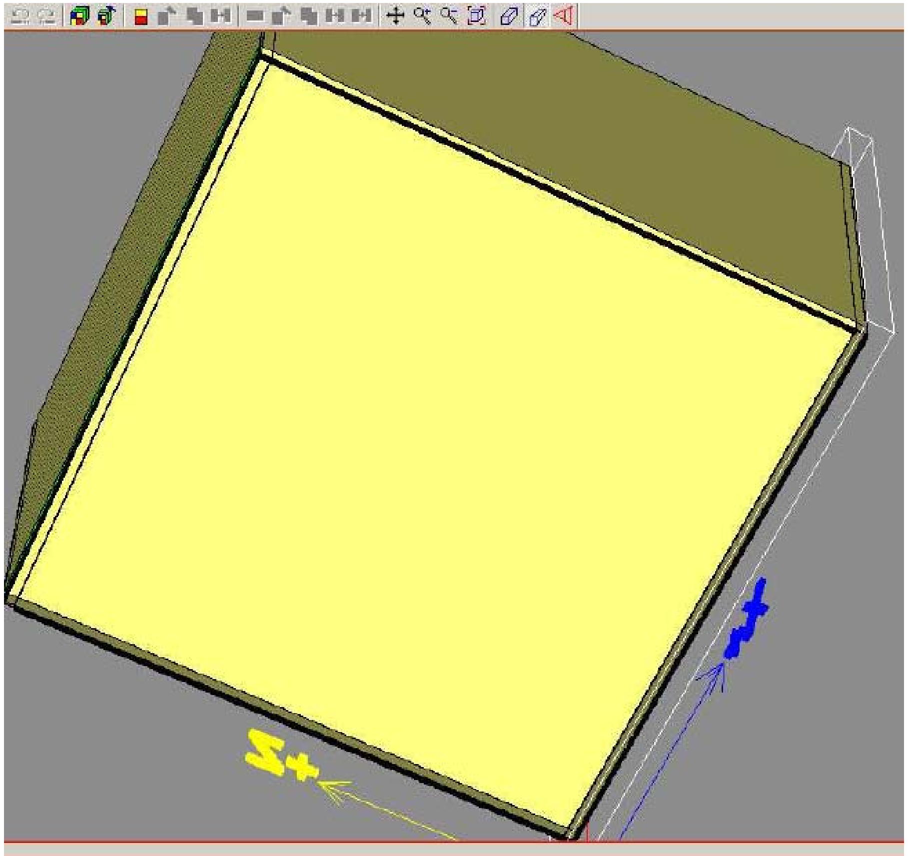
- **Density profiles for acceptor & donor generated from CSuprem.**

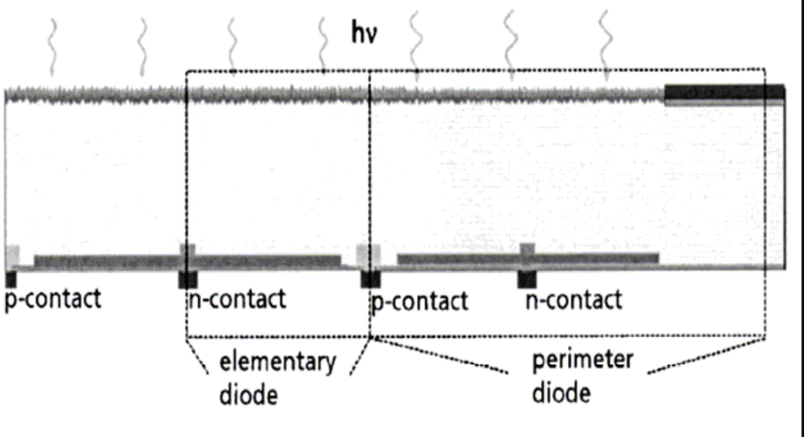
I-V curve with CSuprem doping profile



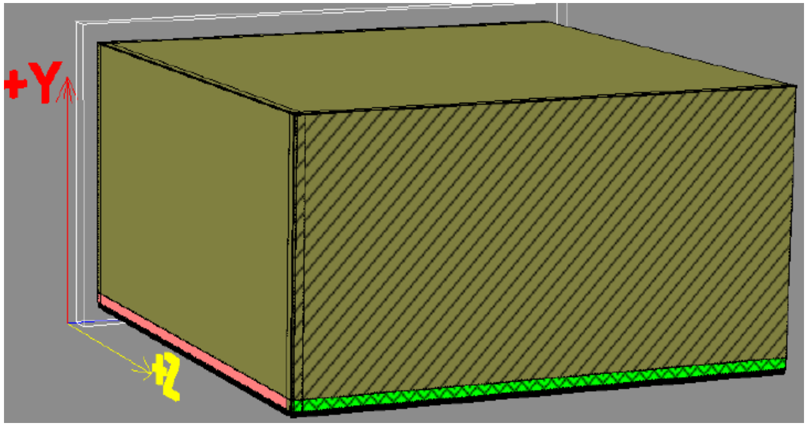
- **With imported doping profiles & with triangle textured surface & coating at front top.**

3D Si RCC modeling



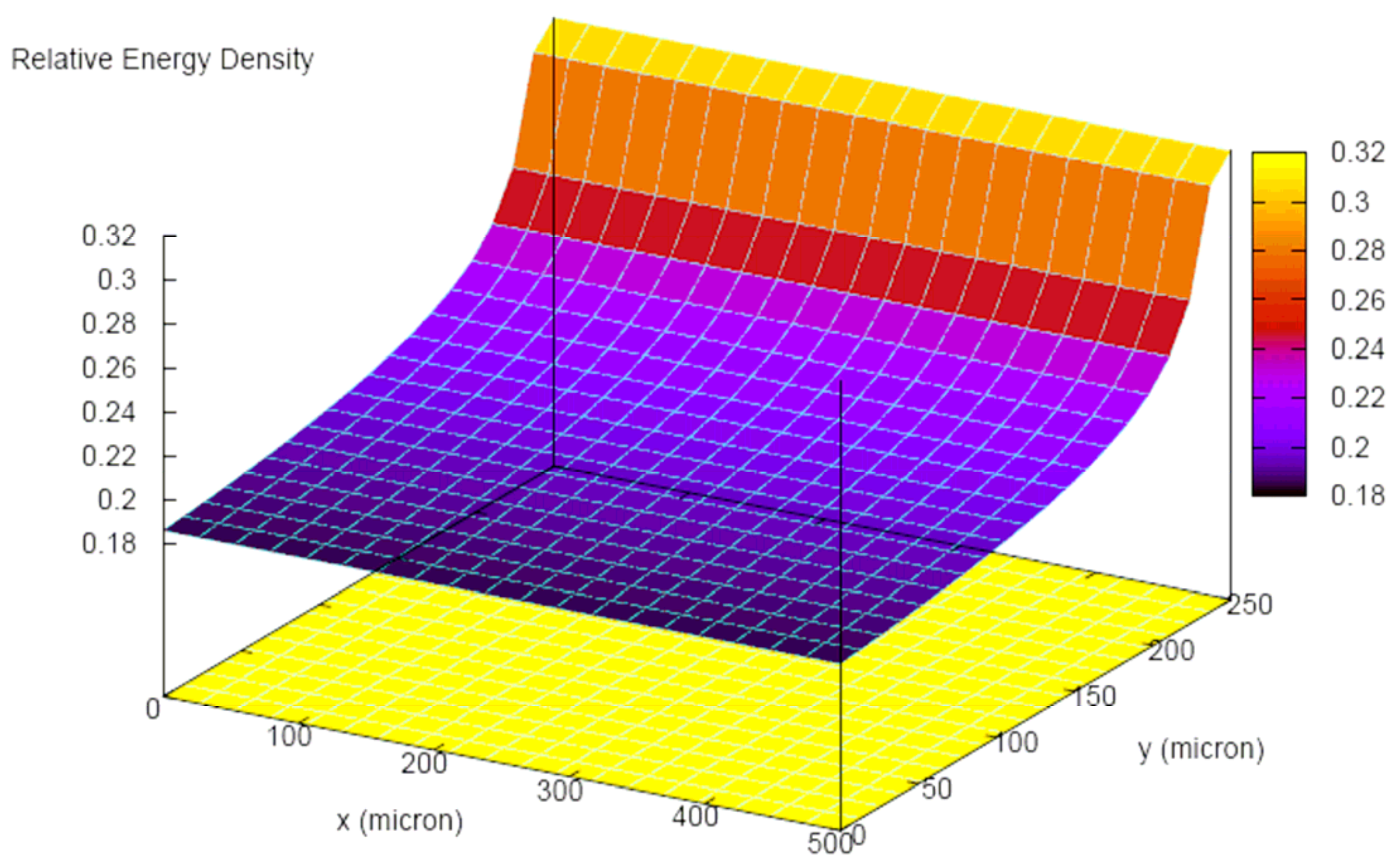


J Dicker et al, JAP, V91N7, 2002, pp4335-4343



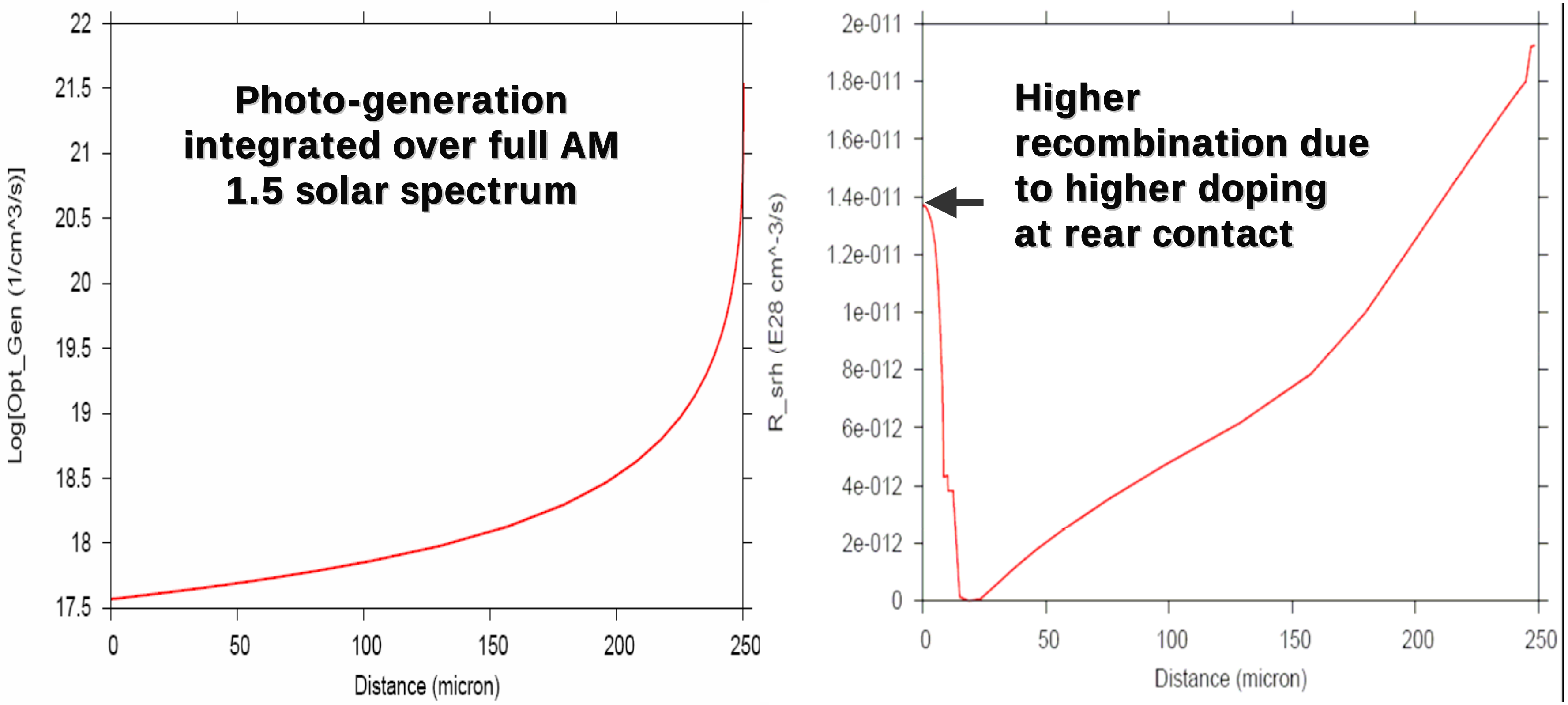
- **Setup of 3D device structure with Crosslight layer 3D for full 3D simulation.**

Light power density within 3D RCC



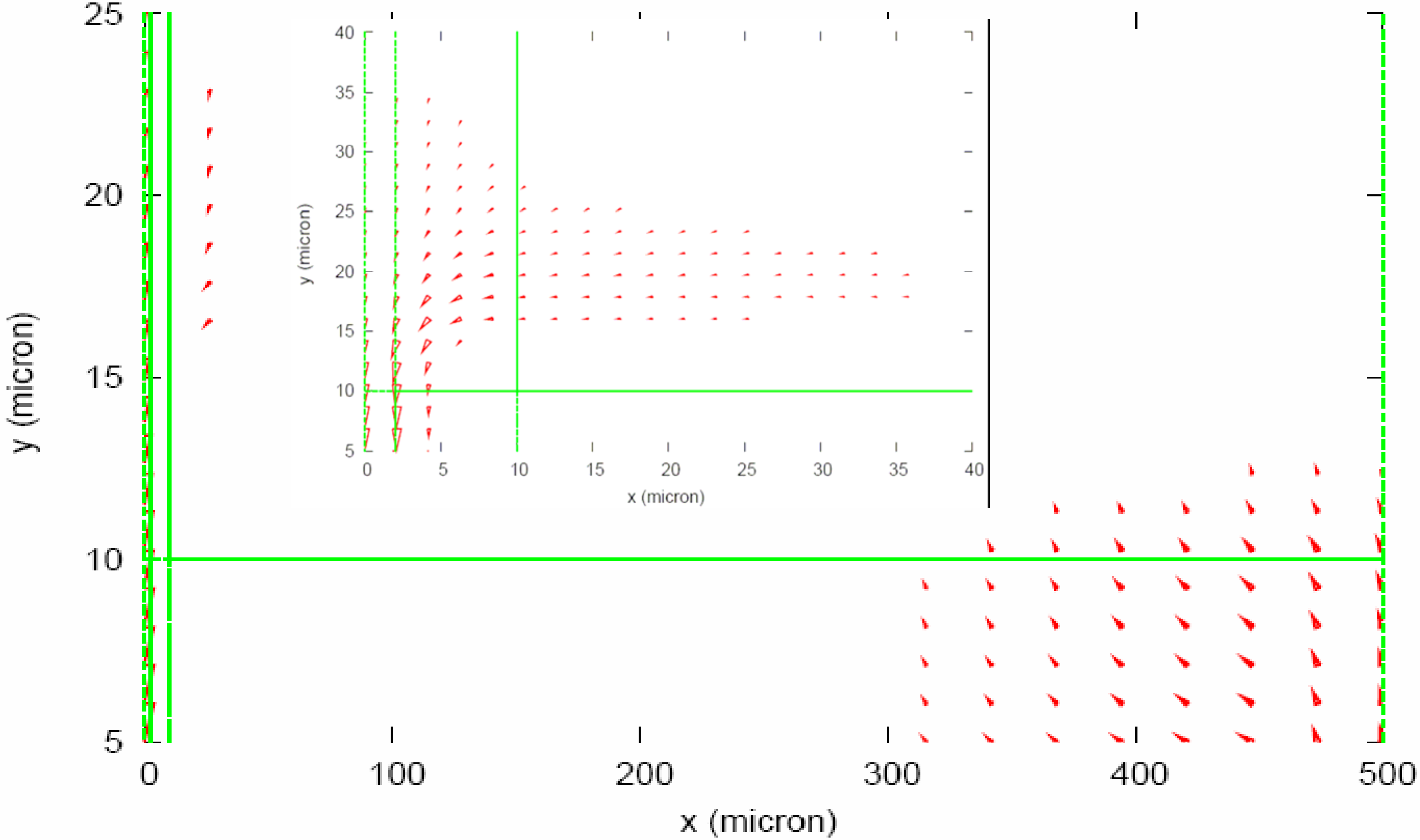
- **Solar absorption (total absorption thickness 250 μm). AM 1.5 illumination assumed. Intensity integrated over full spectrum. 100 nm SiO_2 coating at the front surface.**

Generation & Recombination – 3D RCC



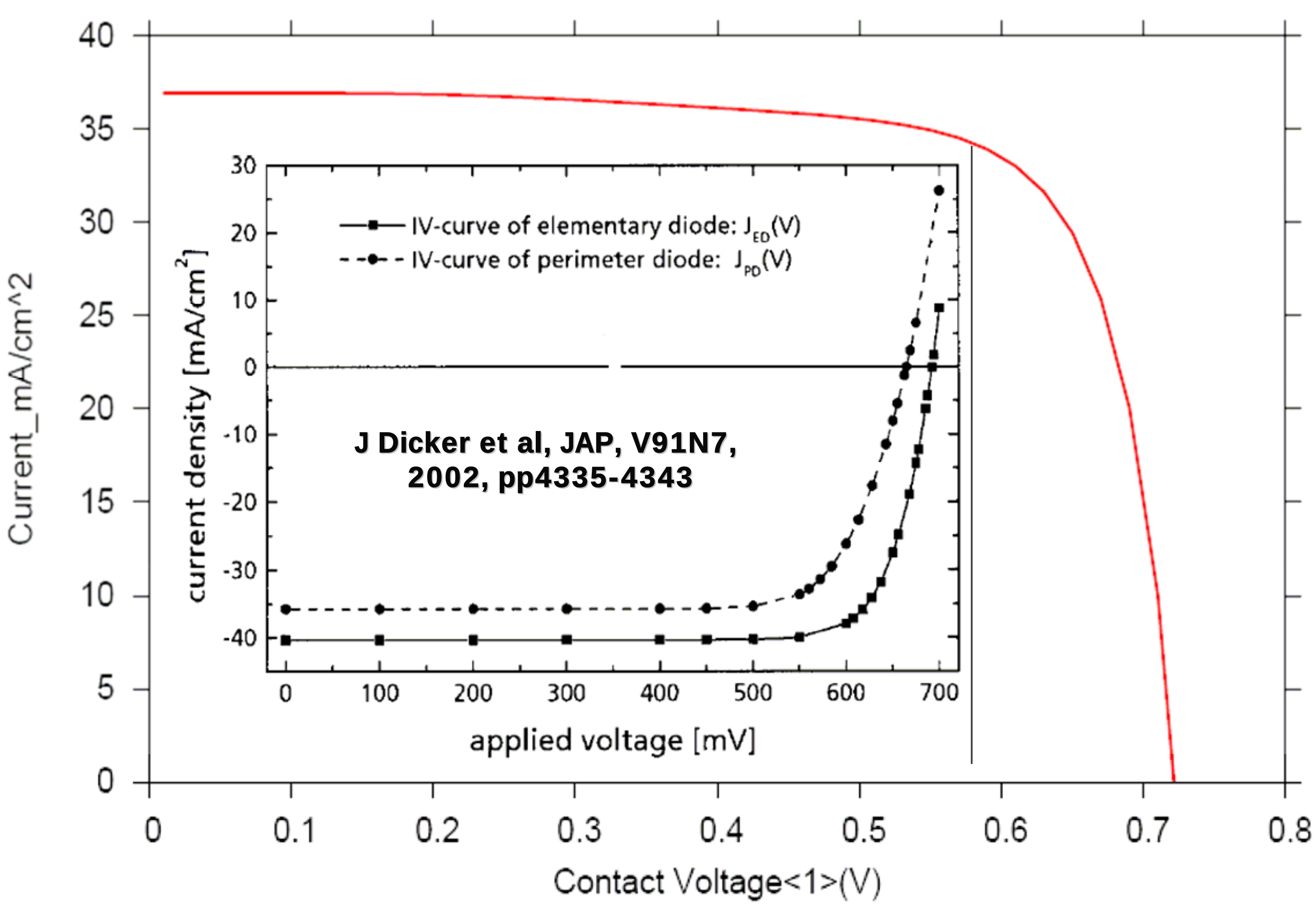
Sunlight direction

Current flow – 3D RCC



- **Current flow at cross-section (portions) for middle z-regime.**

Comparison with experiment – 3D RCC



- **I-V curve with Voc at around 0.72V & Isc about 37.0 mA/cm², in agreement with the experimental results.**

SunPower's RCC structure

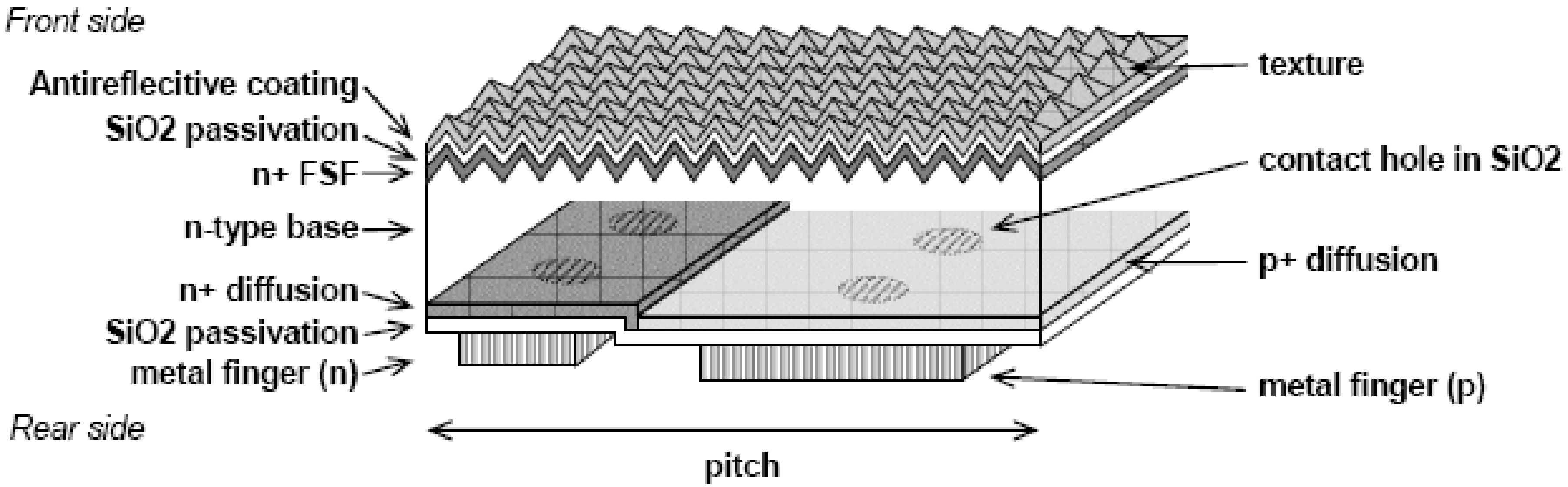
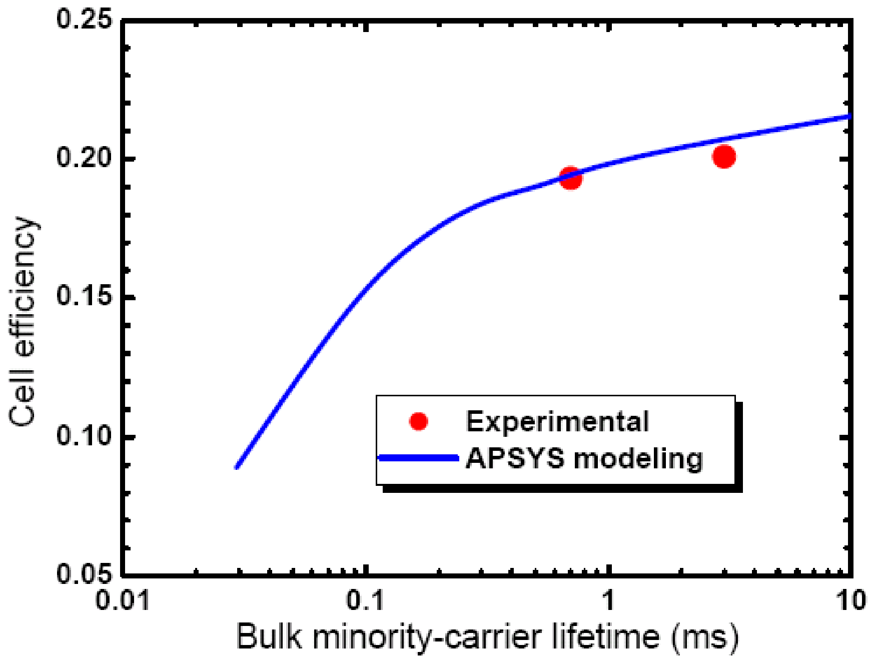


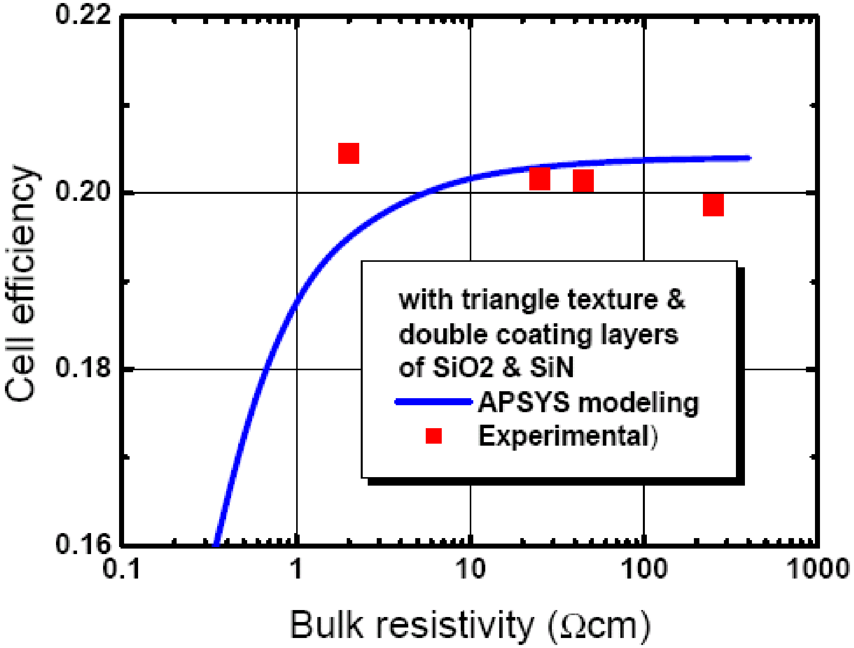
Figure 1: Schematic diagram of SunPower's low-cost rear-contact solar cell (not to scale).
NB: This diagram depicts an *n*-type base, but it could equally well be a *p*-type base.

Ref: Keith R. McIntosh et al, "The choice of Silicon wafer for the production of low-cost rear-contact solar cells," in Proceedings of 3rd World Conference on Photovoltaic Energy Conversion, 2003, vol. 1, pp 971-974.

- **Triangle texture handled by ray tracing separately.**

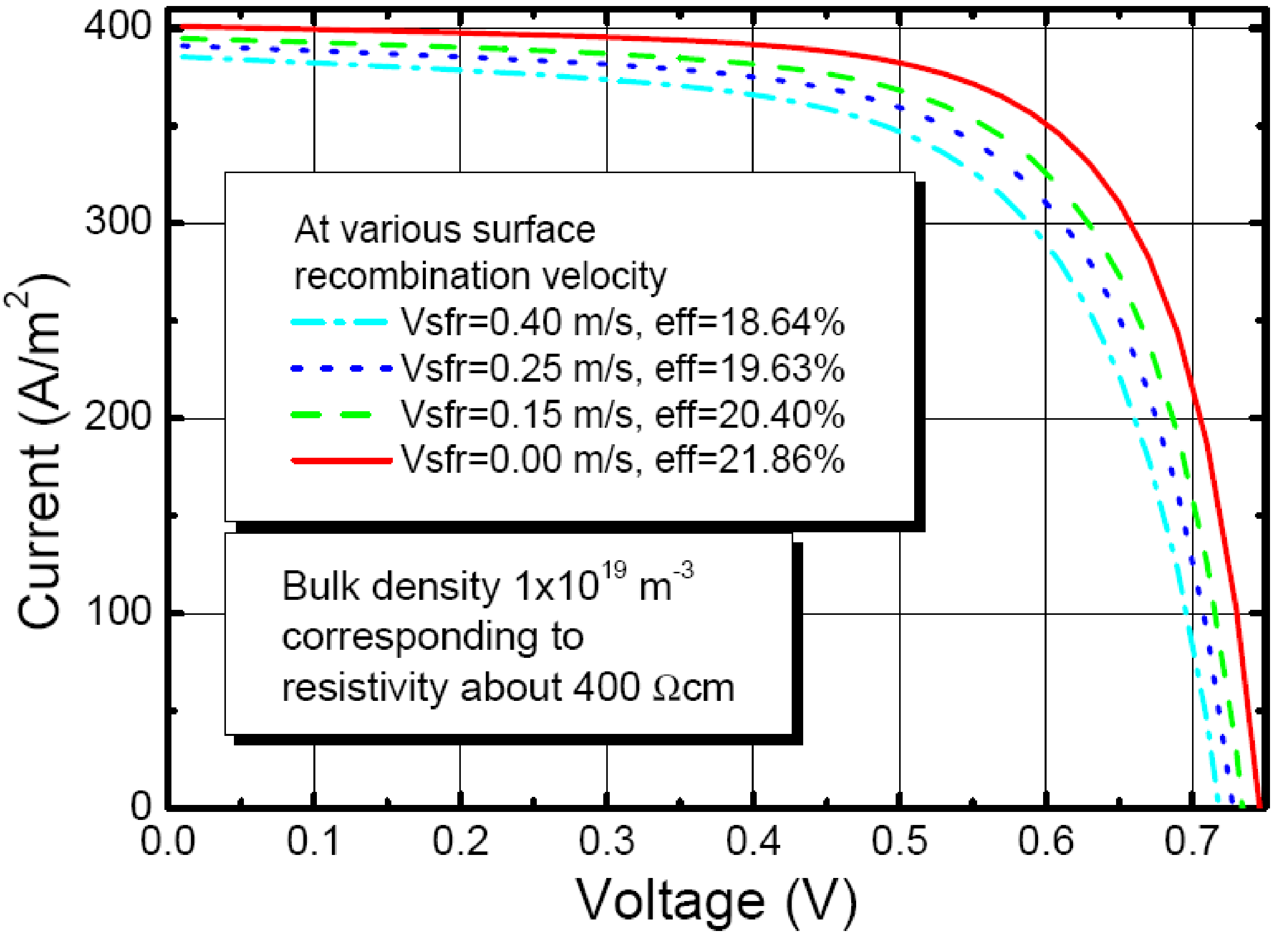
Results comparison





- **Results in general agreement with experimental. Also consistent with results of other simulator.**

Effect of surface recombination



- **High cell efficiency achieved as long as surface recombination could be effectively suppressed.**

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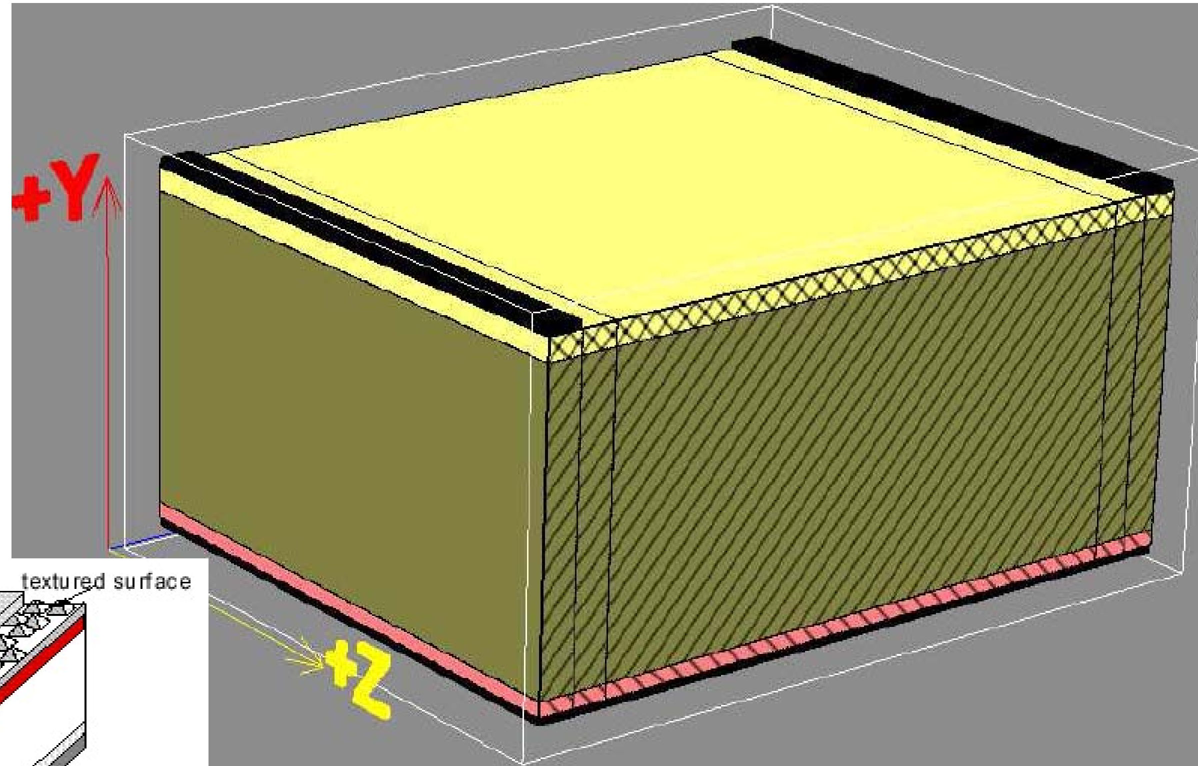
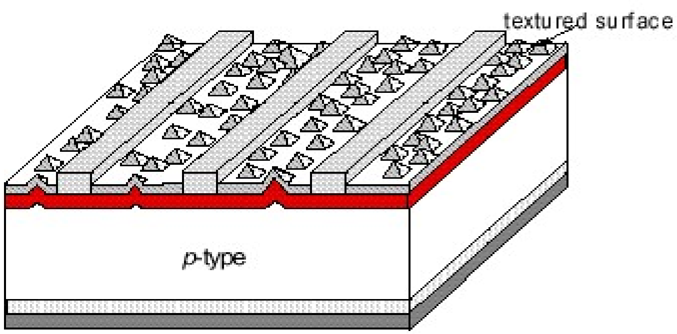
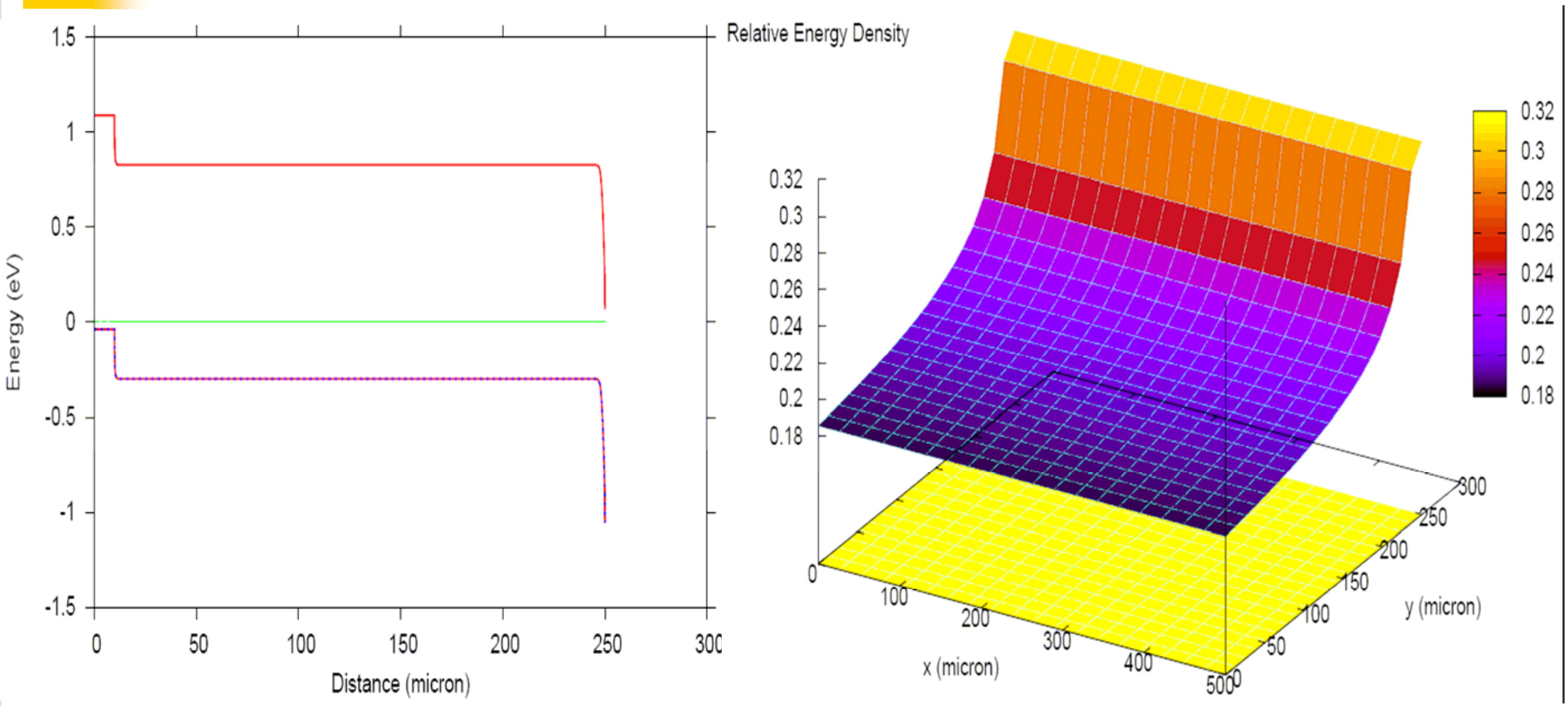
3D PERT cell – surface n contact





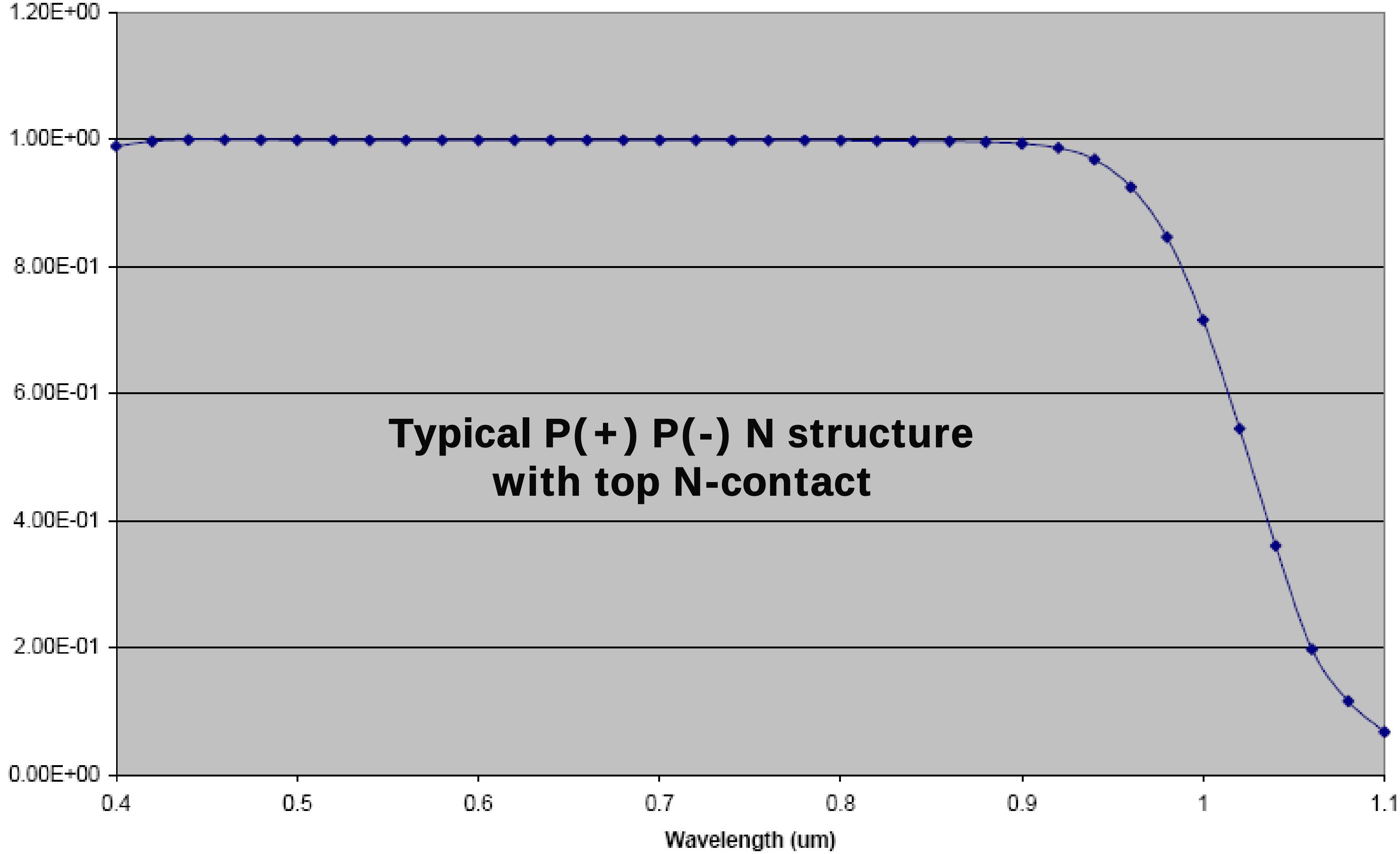
- **Setup of 3D device structure with Crosslight LayerBuilder (bottom totally diffused p^+ / middle lightly-p / top n^+, device xy size 250x500 μm^2).**

Band diagram & light power density



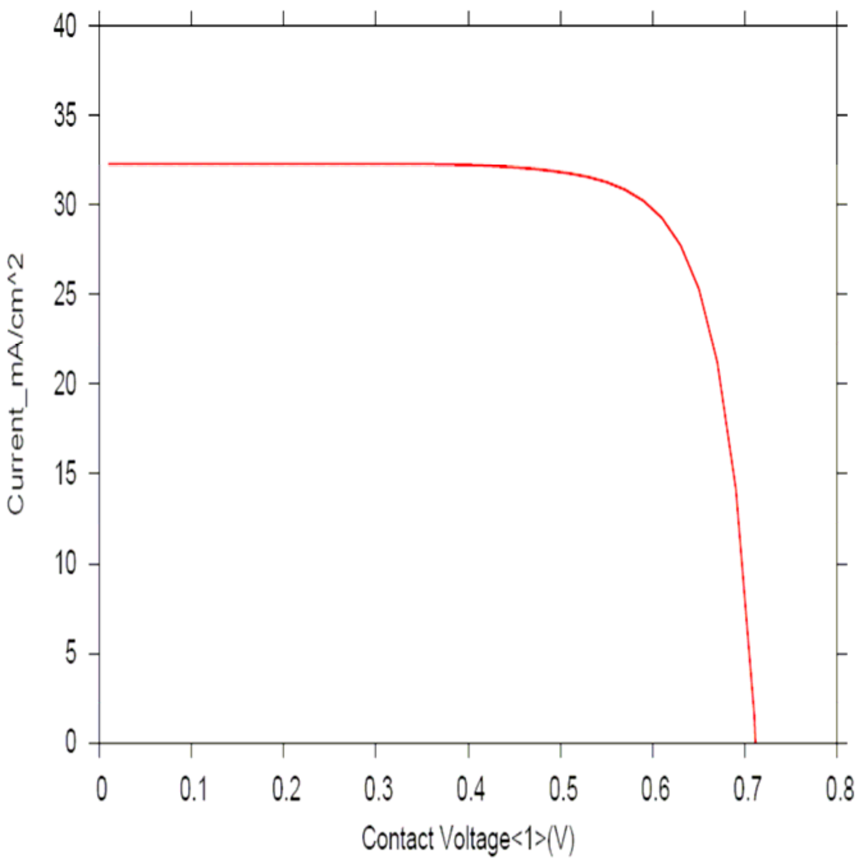
- **Band diagram at equilibrium (assuming 240 μm for the middle p-layer, cut through middle x along y).**
- **Relative energy density distribution, illumination from top at large y-value. Energy density decreases more for thick p-layer.**

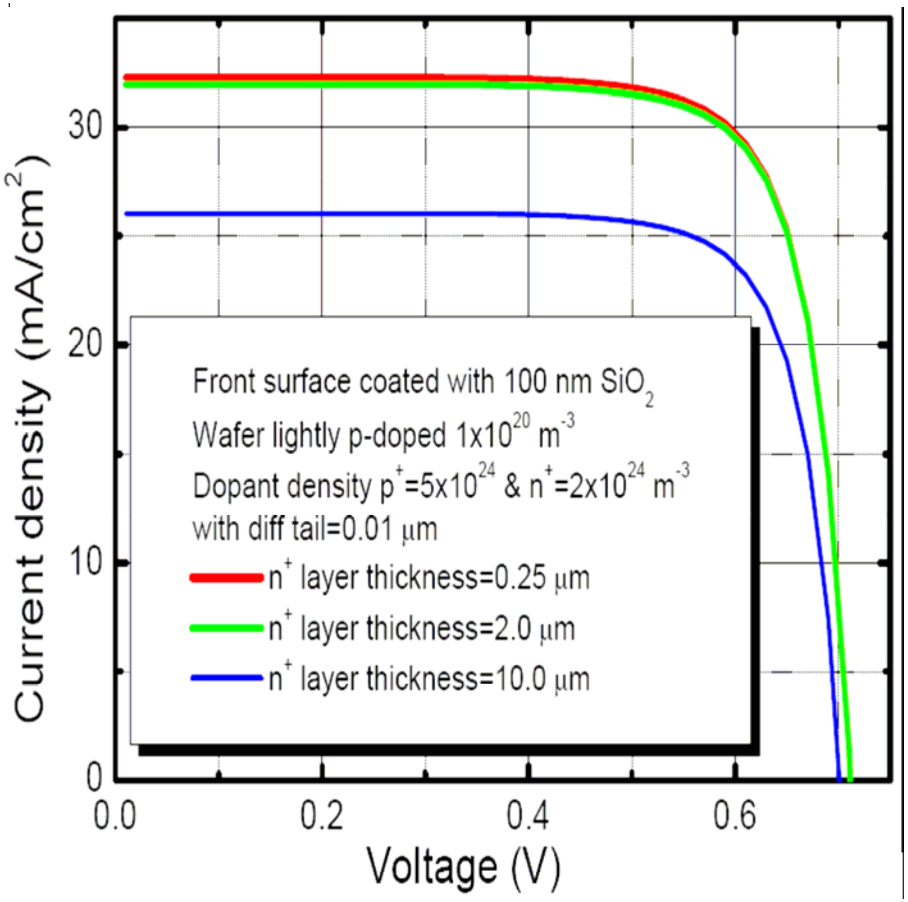
Typical simulated IQE



Remark: Simulation series were set from GUI to scan wavelength to compute short circuit current → IQE

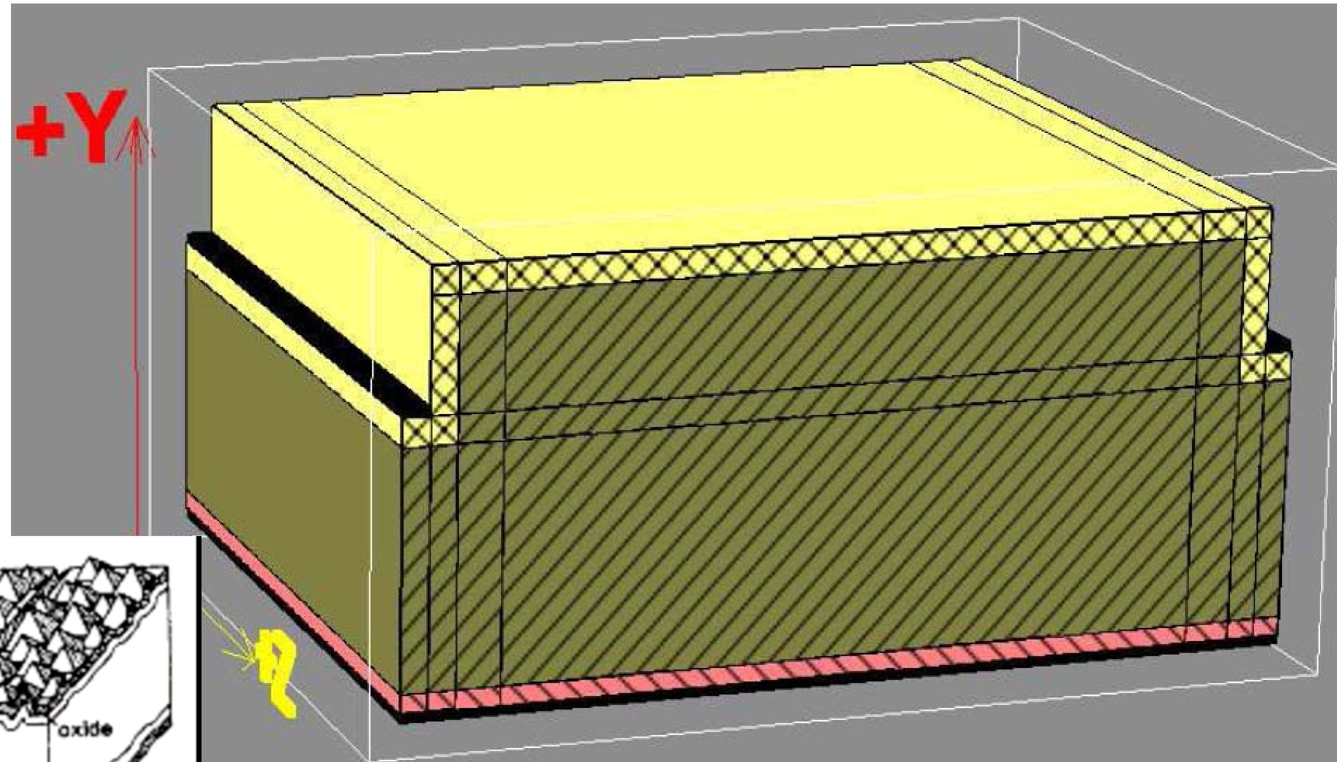
I-V curve

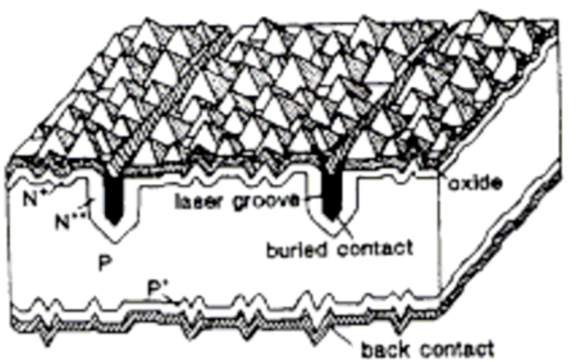




- **I-V curve (240 μm for the middle p-layer). For contact pads on both sides, thick middle (light doped) p-layer with very thin emitter n^+ layer (~0.25 μm) is preferred.**

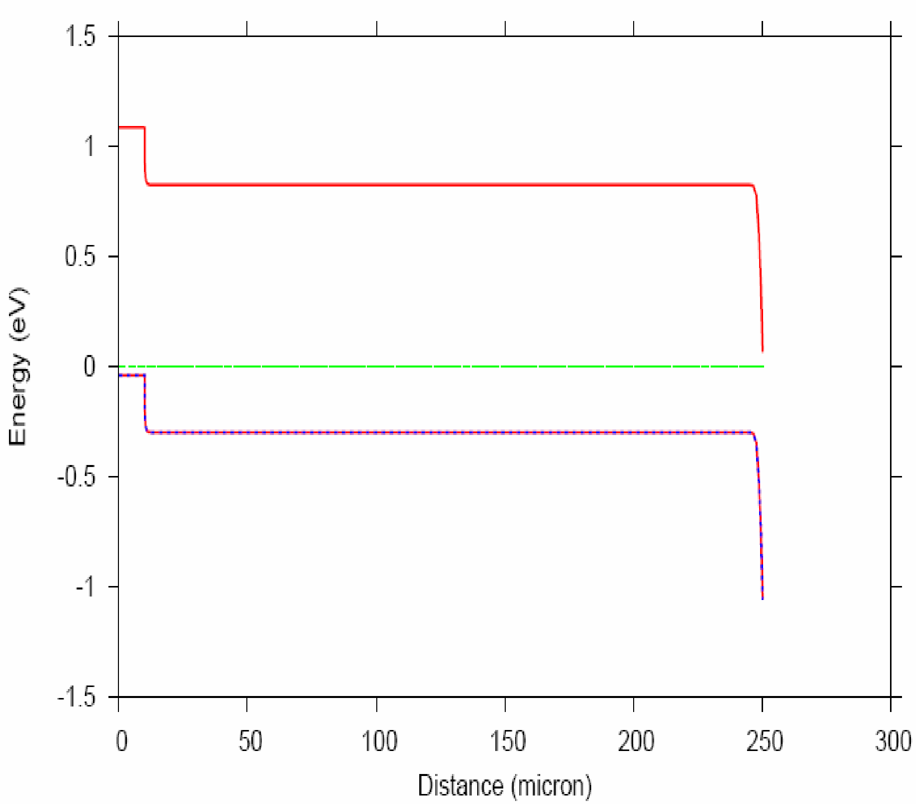
3D PERT cell – buried n contact

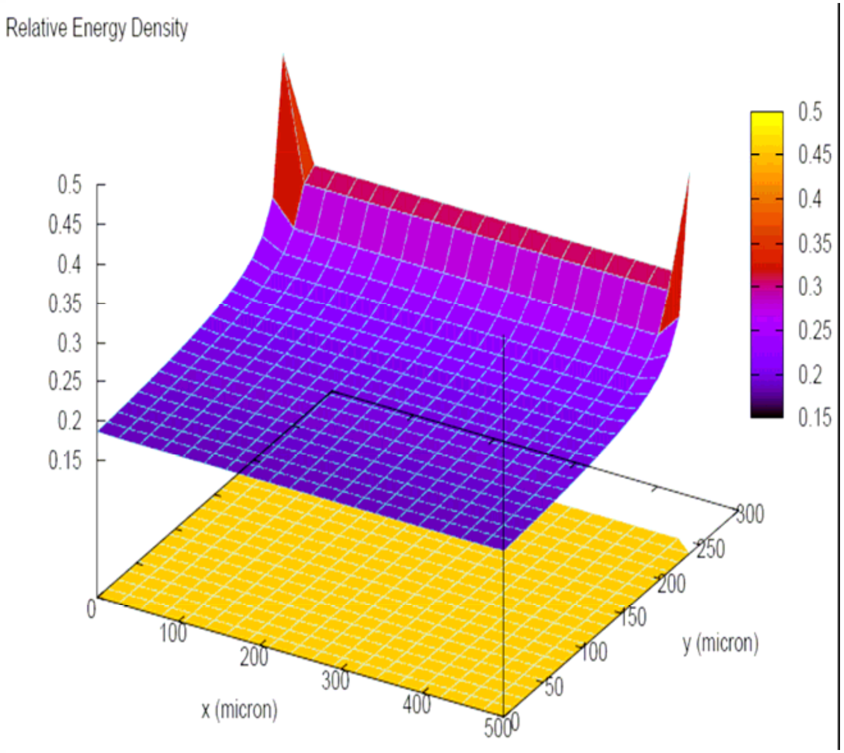




- **Setup of 3D device structure with Crosslight LayerBuilder (bottom totally diffused p+ / middle p / top n+, assuming total middle p-layer 240 μm, grooving depth into the middle p-layer around 10 μm, device xy size 250x500 μm²).**

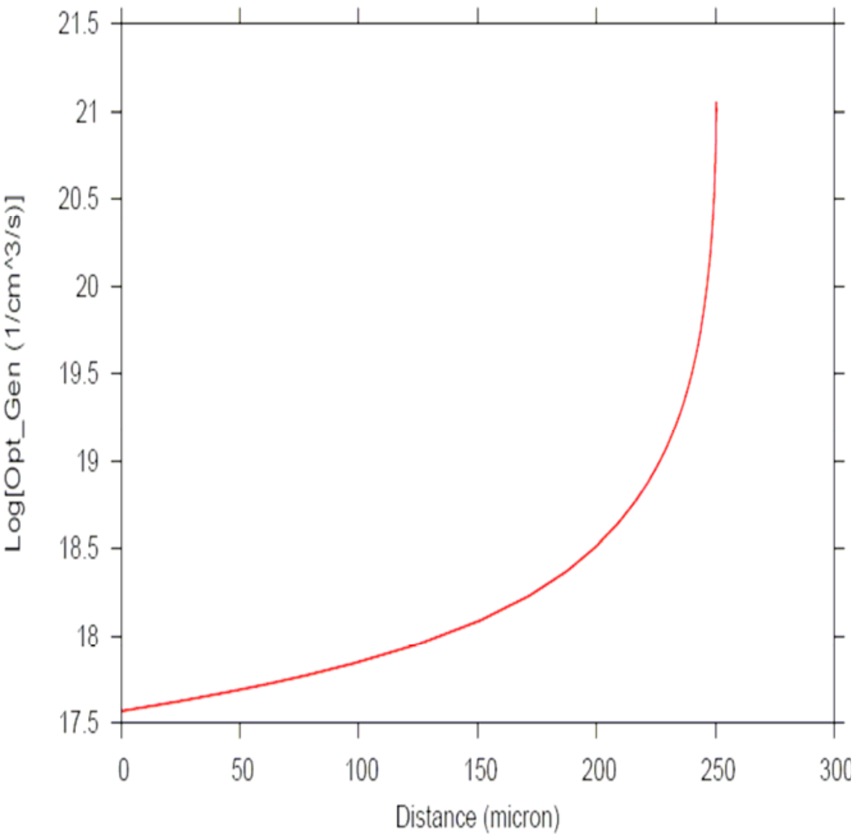
Band diagram & light power density

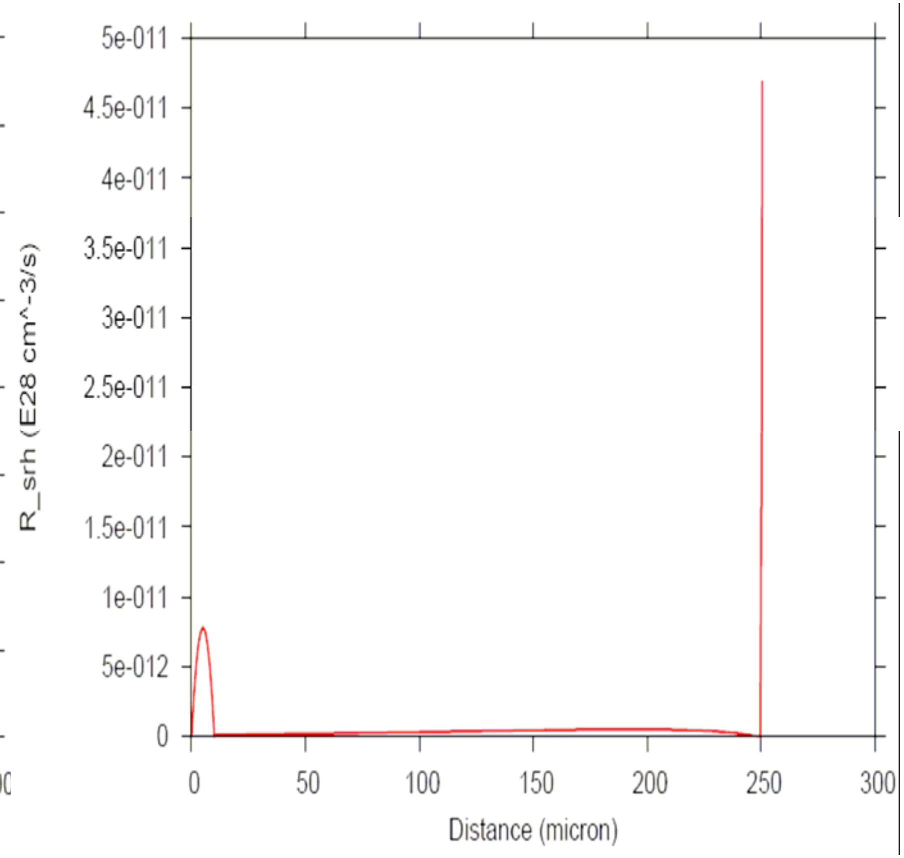




- **Band diagram at equilibrium (cut through middle-x along y).**
- **Relative energy density distribution, illumination from top (corresponding to large y-value).**

Generation & recombination

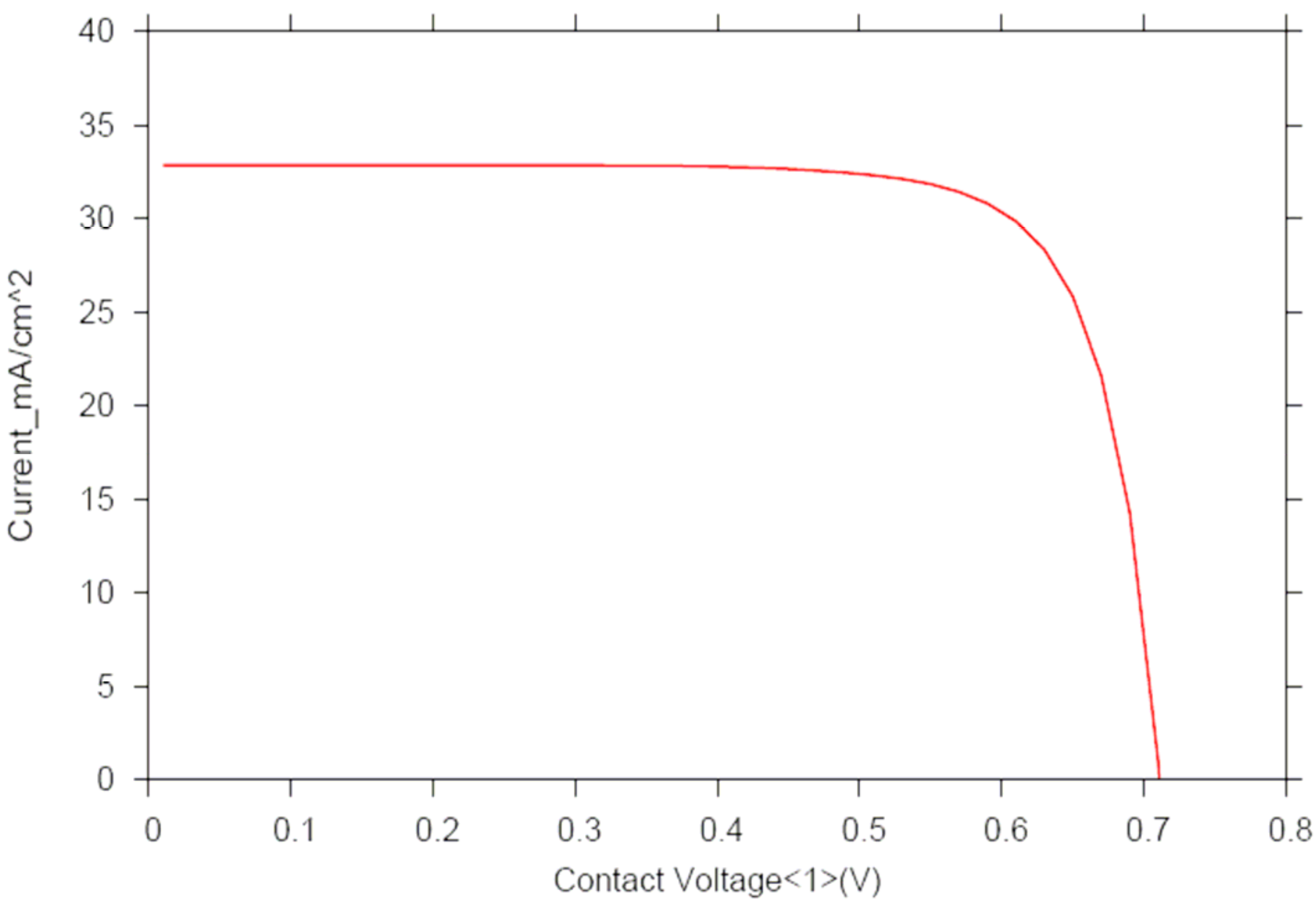




Optical generation rate.

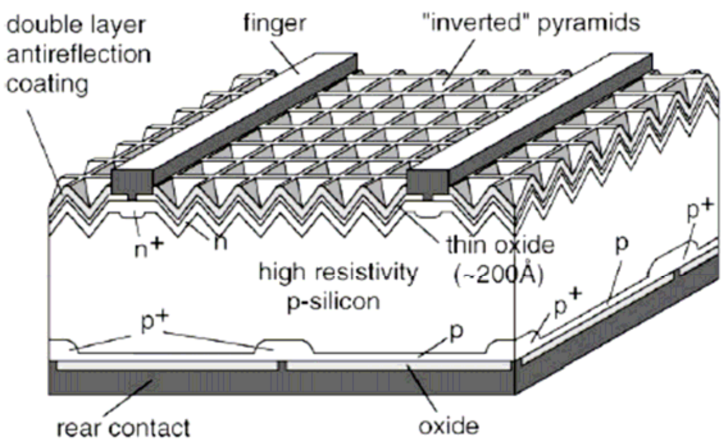
SRH recombination , under solar illumination, short circuit case.

I-V curve

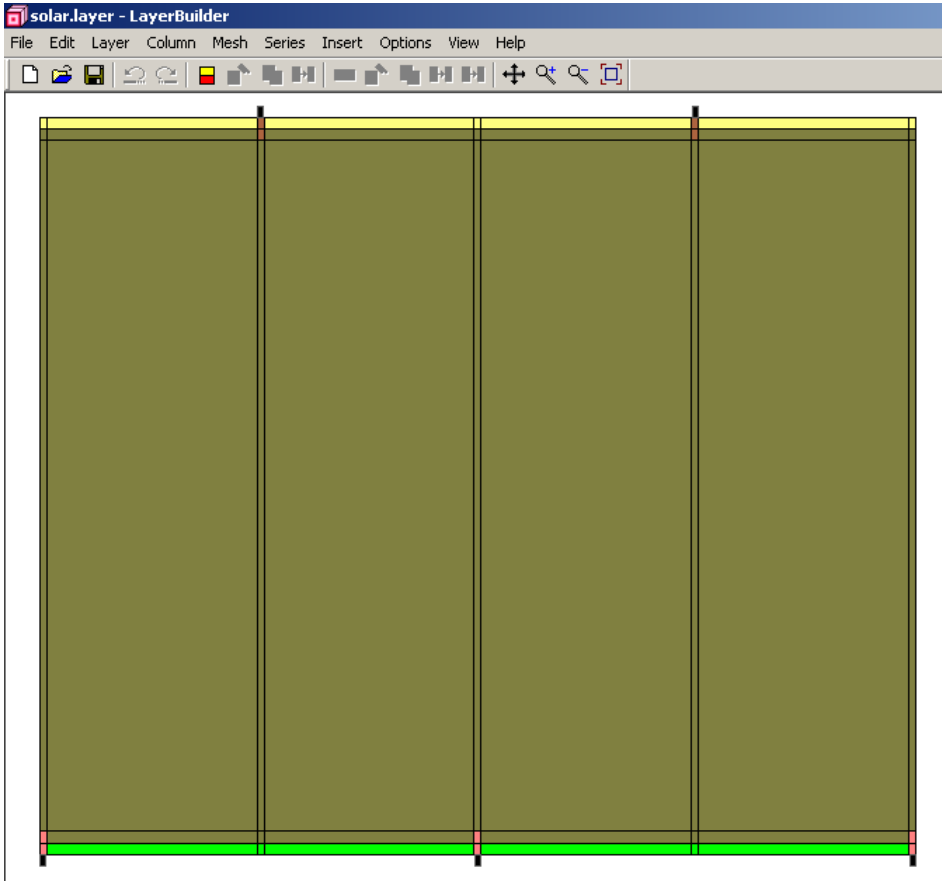


- **I-V curve. For contact pads on both sides, thick middle (light doped) p-layer is preferred.**

PERT cell with record efficiency

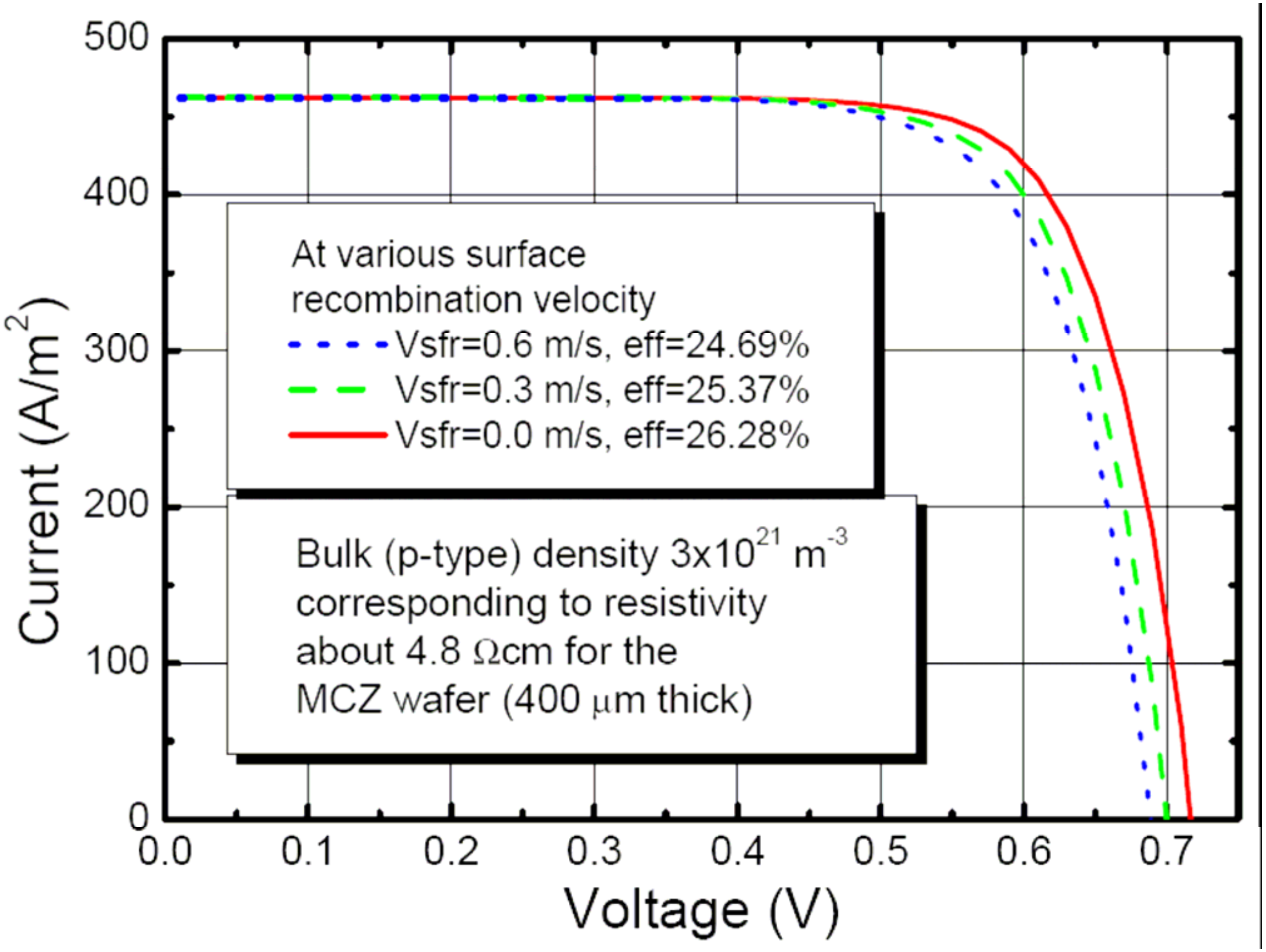


Ref: **JH Zhao et al, "24.5% efficiency PERT silicon solar cells on SEH MCZ substrates and cell performance on other SEH CZ and FZ substrates," Solar Energy Materials & Solar Cells 66 (2001) 27-36.**



- **Setup of 2D device structure with Crosslight LayerBuilder.**
- **Triangle texture handled by ray tracing separately.**

2D modeling I-V curves



Summary

- **Crosslight's flexible material database (user accessible macros) makes it easy to implement Si & poly-Si mobility & lifetime as a function of doping and grain size.**
- **Device simulation is fully integrated with process simulation.**
- **Si rear-contacted cells (RCC) simulated with results in agreement with experiment.**
- **When combined with Crosslight's 2D / 3D ray tracing module, complex solar cell structures with textured surface may be treated.**
- **PERT cell devices with front surface n contact & with buried n contact together with texture and coating simulated and results are selectively demonstrated.**