Applying technology computer aided design (TCAD) to performance improvement of silicon wafer solar cells

Never Stand Still | Faculty of Engineering | School of Photovoltaic and Renewable Energy Engineering

Speaker: Dr. Fa-Jun MA

Time: 1200 – 1300

Date: 28th May 2015

Location: TETB LG07

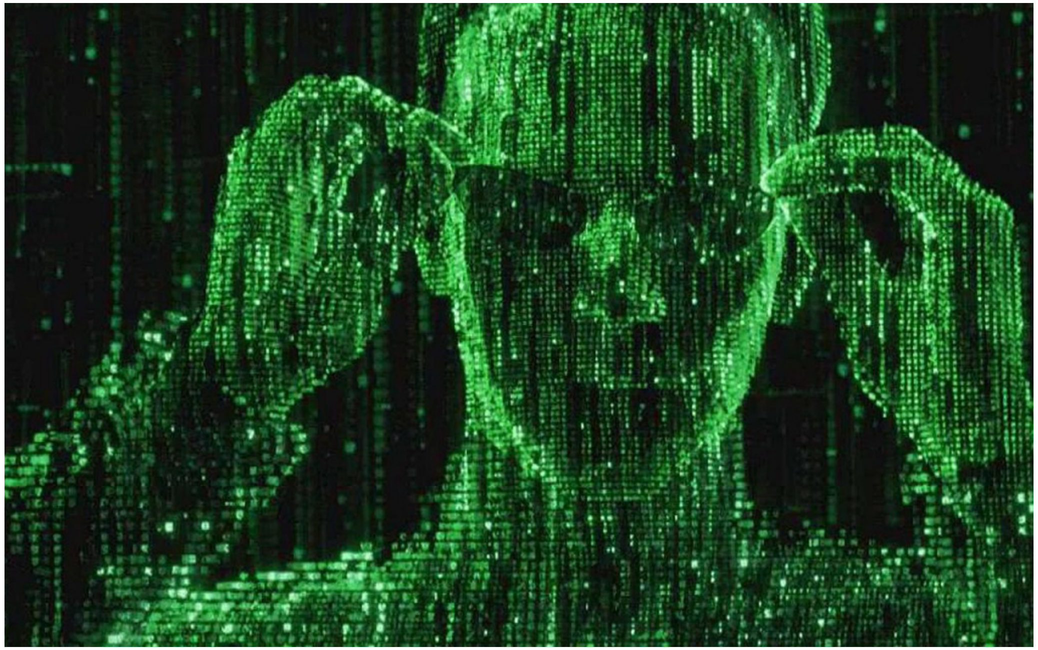
Are we familiar with simulation?

- We all did simulation since childhood!
- With concrete objects, a child learns the world by simulation, where he or she
  - Role plays
  - Experiments
  - Discovers
  - …

Toy blocks for "little architects"

What is computer simulation?

- ❑ It is simulation carried out in a digital world!
- ❑ Computer simulation typically features
  - ➢ Advanced visualization
  - ➢ Artificial objects
  - ➢ Mathematical models
  - ➢ Numerical computation



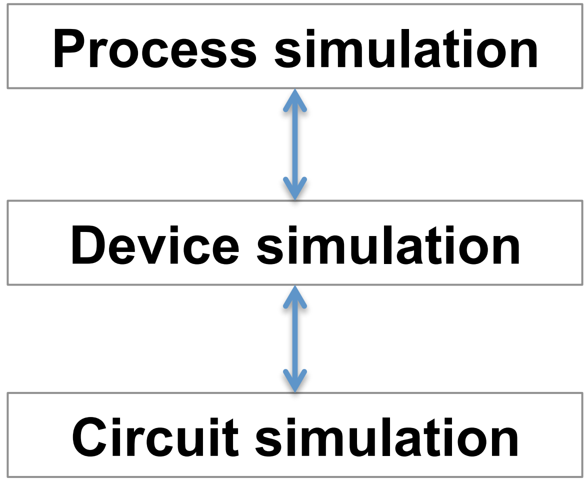
The ultimate computer simulation to live in: The matrix!

Why do we need computer simulation?

- ❑ Computer simulation is widely applied to multiple fields
- ❑ These facts may contribute
  - ➢ A system is very complex with may variables
  - ➢ A system contains random variables
  - ➢ Simulation is more cost effective
  - ➢ An experiment is too dangerous
  - ➢ An experiment is impossible
  - ➢ …

What is TCAD?

- ❑ TCAD is a bundle of up to 3D simulators for predicting semiconductor behaviors in
  - ➢ Complex semiconductor fabrication processes
  - ➢ Complex electrical, optical and thermal device operations
  - ➢ Circuit simulation
- ❑ TCAD is matured enough to provide reasonable accuracy



Outline

- Enumeration of the benefits of TCAD involvement in solar research
  - Gaining insights
  - Making yourself understood
  - Revealing the underlying physics
  - Discovering new phenomena
  - Predicting performance improvement
  - Deterministic modelling
  - Inverse modelling
  - Compact modelling
  - …
- Summary

Advantages of commercial packages

- Examples in this talk were simulated with Sentaurus TCAD [1]
- The advantages are
  - Multi-dimension
  - Multi-physics
  - Multi-device
  - Multi-material

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Synopsys, Inc., an American company, is the leading company by sales in the Electronic Design Automation industry. Synopsys' first and best-known product is Design Compiler, a logic-synthesis tool. Wikipedia

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CEO: Aart de Geus

Headquarters: Mountain View, CA, United States of America

Founded: 1986

Founders: Alberto Sangiovanni-Vincentelli, Aart de Geus

SILVACO

Silvaco

Company

Silvaco, inc. is a privately owned provider of electronic design automation software and TCAD process and device simulation software. Wikipedia

Headquarters: Santa Clara, CA, United States of America

Founded: 1984

Gaining insights

- ❑ Abstract thinking may not help you gain insights as
  - ➢ Partial differential equations are difficult to understand
  - ➢ Many variables are interacting with nonlinear relationships
  - ➢ A closed-form solution may not exist
- ❑ Simulation is much easier and more helpful comparing to abstract thinking

$$\nabla(\varepsilon_0 \varepsilon_s \nabla\phi) = -q(p - n + N_D - N_A) - \rho_{trap}$$

$$J_n = q\mu_n n\mathrm{E} + qD_n\nabla n = q\mu_n\left(n\mathrm{E} + \frac{kT}{q}\nabla n\right)$$

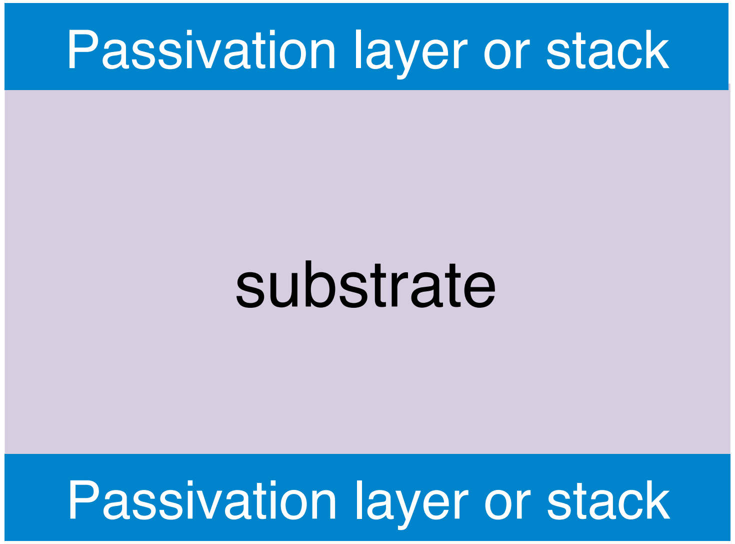
$$J_p = q\mu_p p\mathrm{E} - qD_p\nabla p = q\mu_n\left(p\mathrm{E} - \frac{kT}{q}\nabla p\right)$$

$$\frac{\partial n}{\partial t} = G_n - U_n + \frac{1}{q}\nabla J_n$$

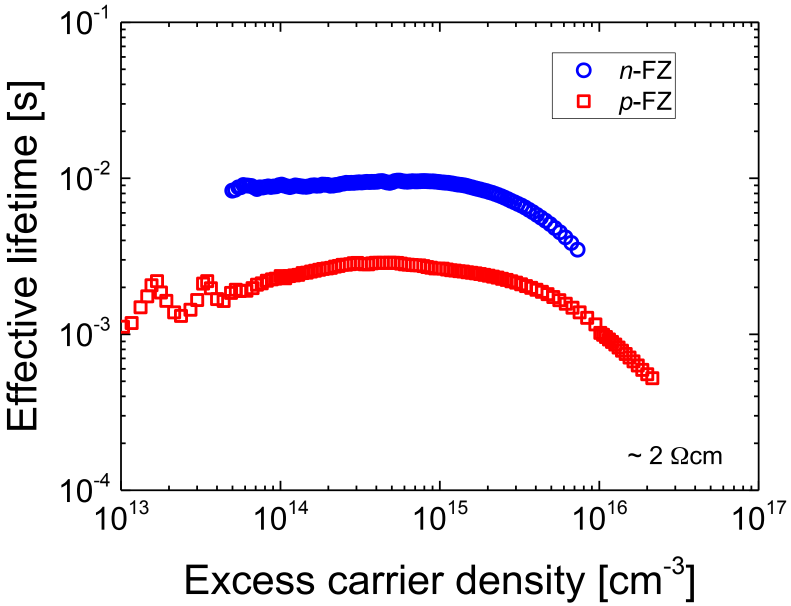
$$\frac{\partial p}{\partial t} = G_p - U_p - \frac{1}{q}\nabla J_p$$

Basic equations governing electrical behaviors of semiconductors

Example: Gaining insights of recombination mechanisms



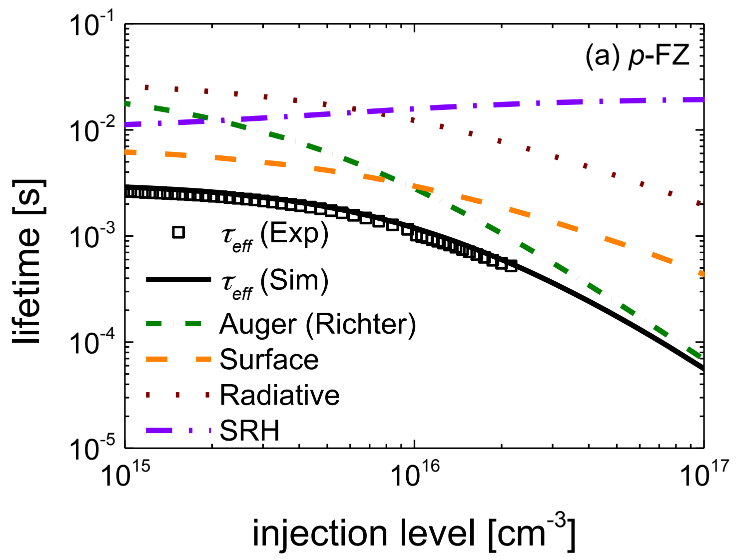
Schematic representation of symmetrically passivated undiffused lifetime samples



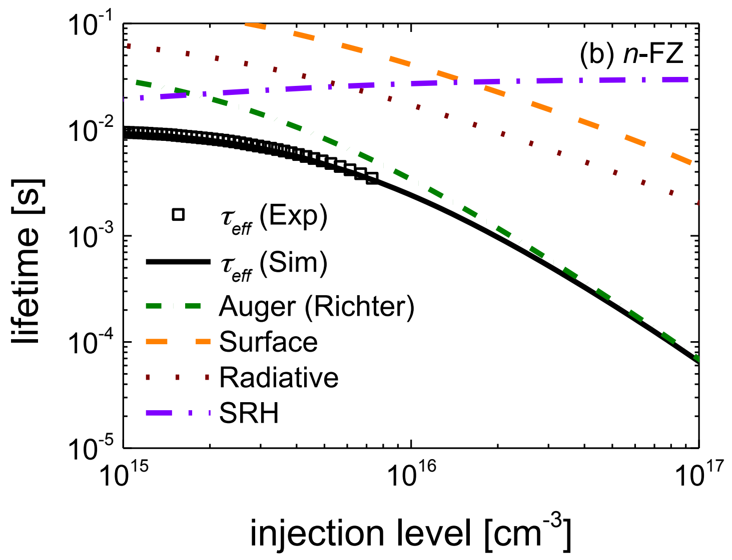
Measured injection dependent effective lifetime curves of undiffused lifetime samples passivated by Al_2O_3 [1]

[1] B. Liao *et al.*, *Journal of Physics D: Applied Physics*, **46**, 385102, 2013.

Example: Dominant recombination at high injection levels



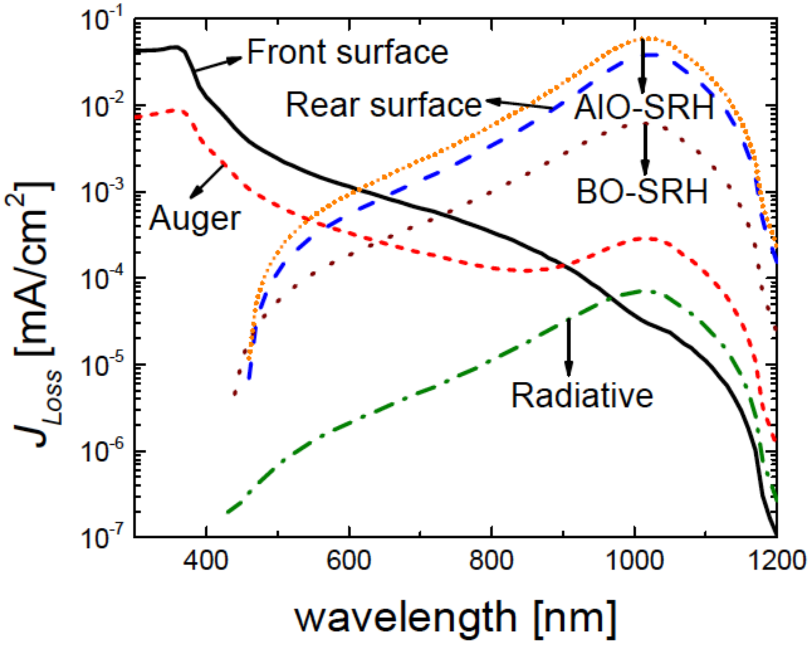
A break down analysis of each recombination for p-FZ [1]



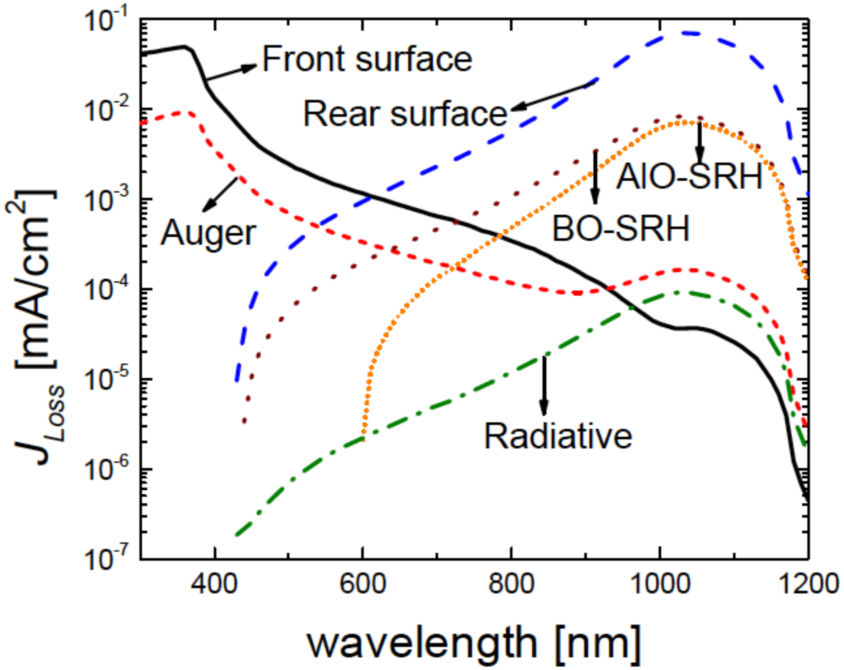
A break down analysis of each recombination for n-FZ [1]

[1] F.-J. Ma *et al.*, *J. Comput. Electron.*, **13**, 647, 2014.

Example: Dominant recombination at different wavelengths in solar cells



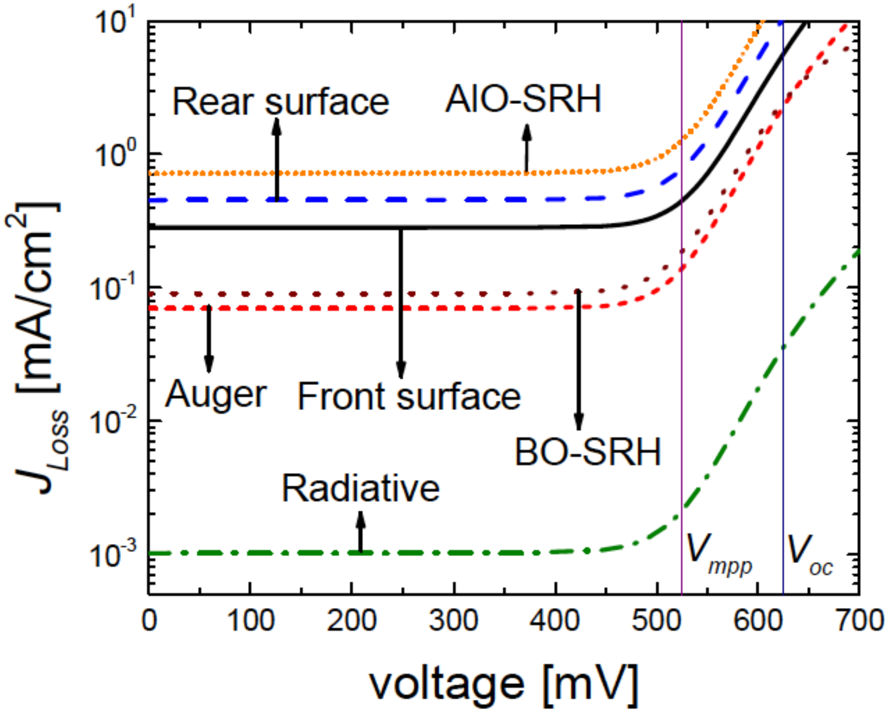
A break down analysis of each recombination at a wavelength range from 300 to 1200 nm for an Al full area BSF solar cell [1]



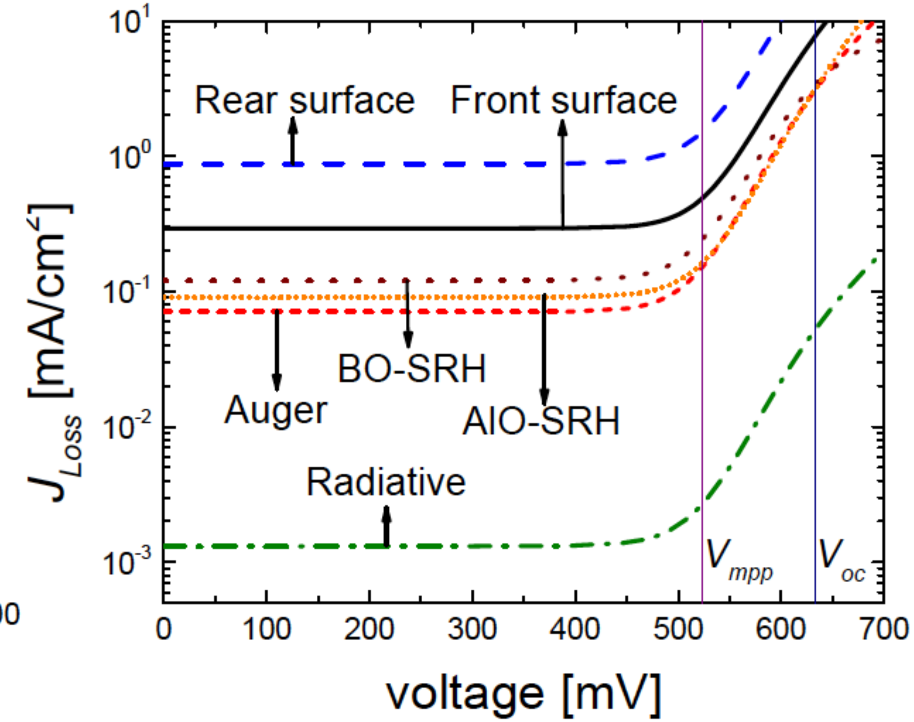
A break down analysis of each recombination at a wavelength range from 300 to 1200 nm for an Al local BSF solar cell [1]

[1] F.-J. Ma, *PhD thesis*, 2014.

Example: Dominant recombination at different bias in solar cells



A break down analysis of each recombination at a bias range from 0 to 700 mV for an Al full area BSF solar cell [1]



A break down analysis of each recombination at a bias range from 0 to 700 mV for an Al local BSF solar cell [1]

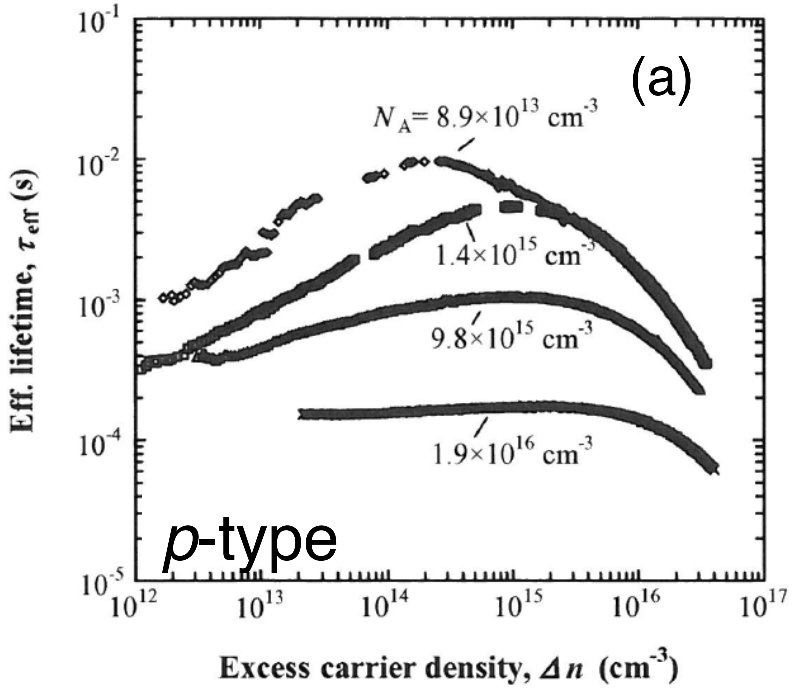
[1] F.-J. Ma, *PhD thesis*, 2014.

Making yourself understood

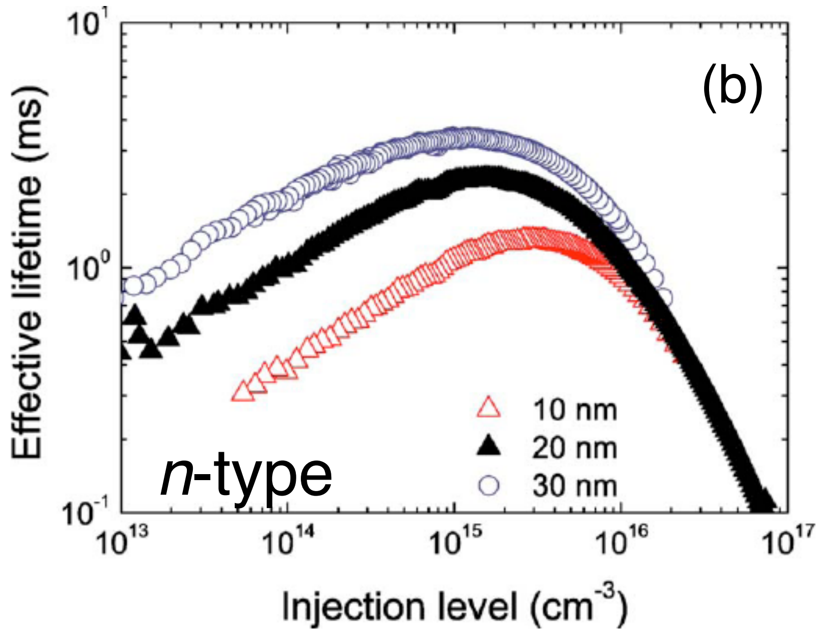
- Most people you interact are not experts in your research
- Presenting lines of theories may not be well conceived
- Advanced visualization from simulation helps spread your insights

Example: Field effect surface passivation

- The effective lifetime under low injection levels is not caused by enhanced surface recombination. How to prove?



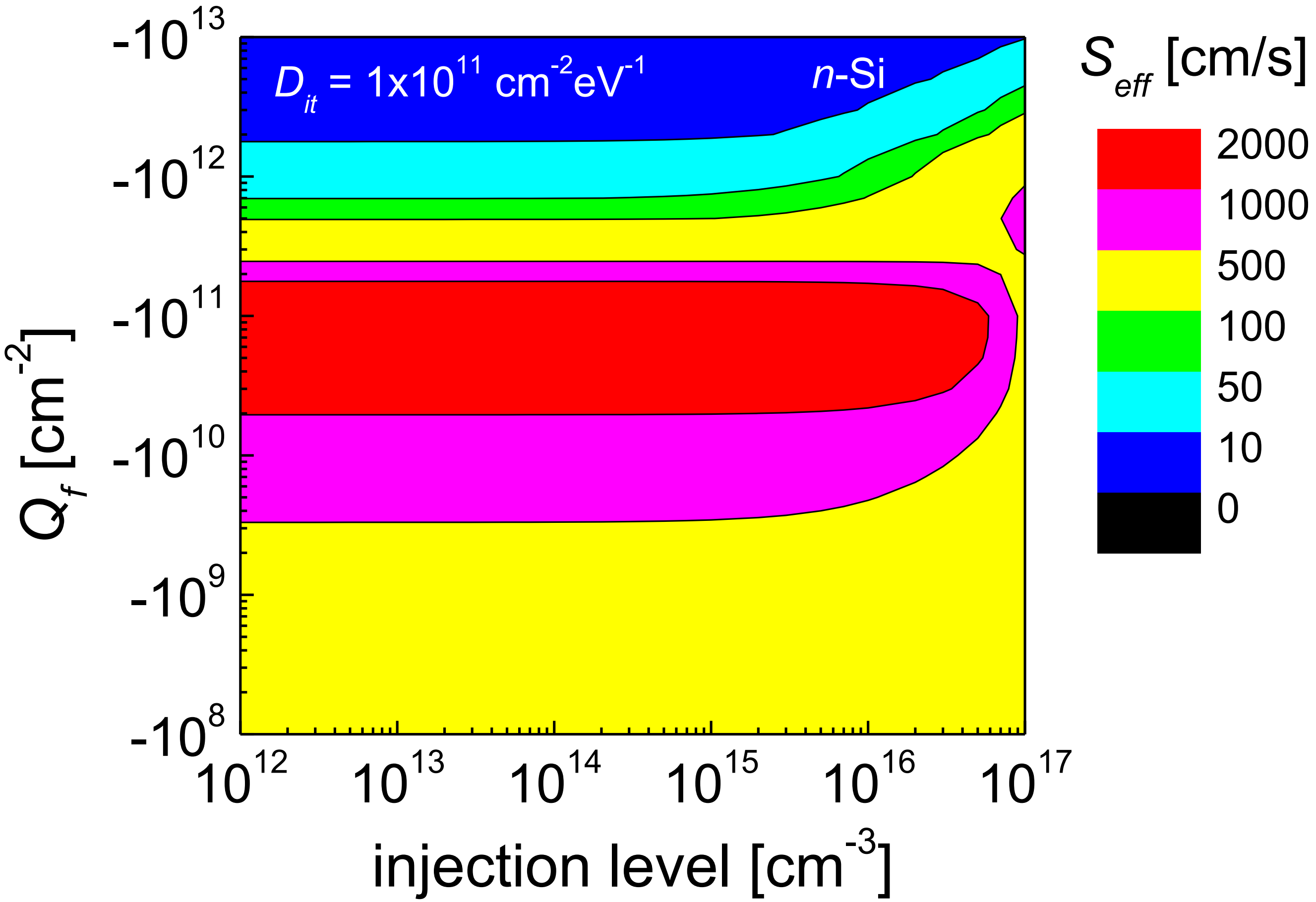
*Measured injection dependent τ_{eff} (passivated by **a-SiN$_x$:H**) [1]*



*Measured injection dependent τ_{eff} (passivated by **Al_2O_3**) [2]*

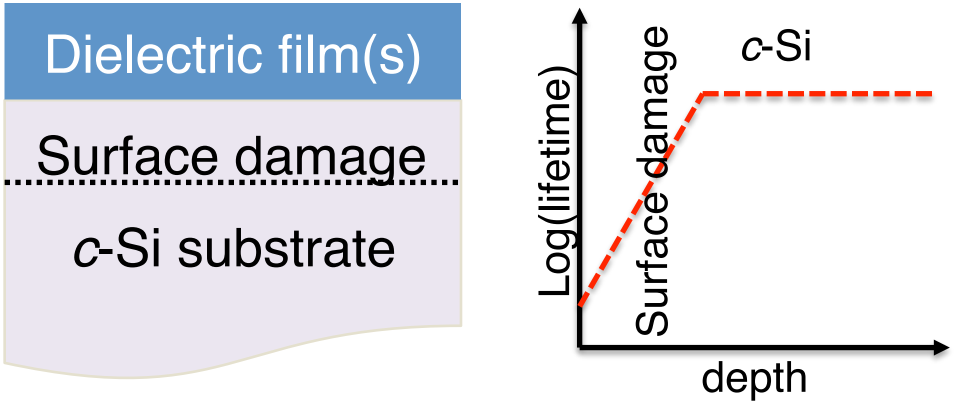
[1] M. J. Kerr and A. Cuevas, *Semicond. Sci. Technol.*, **17**, 166, 2002.
[2] B. Hoex *et al.*, *J. Appl. Phys.*, **04**, 044903, 2008.

Example: Field effect surface passivation

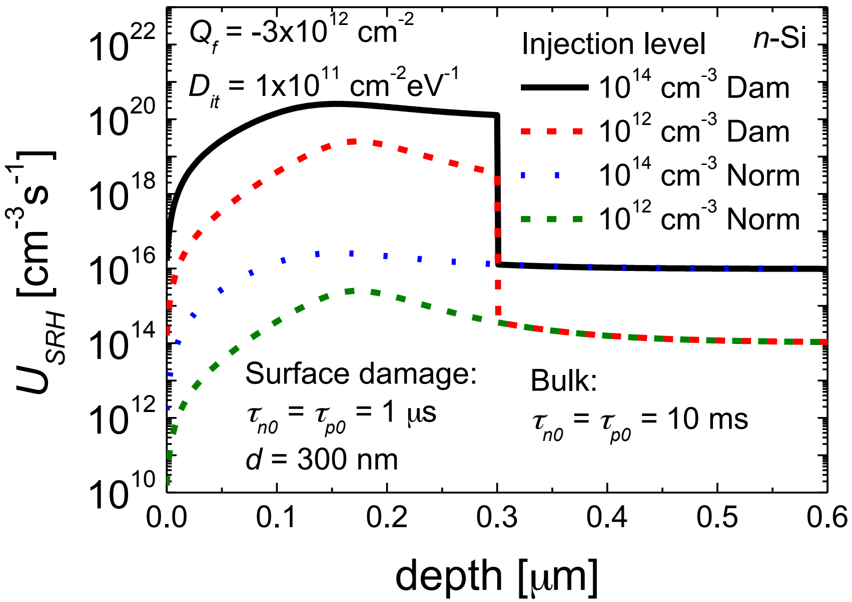


Simulated S_{eff} plotted against the injection level and the negative fixed charge density Q_f for an n-type (N_D 2.5 x 10^{15} cm^{-3}) lifetime sample

Possible mechanisms – damaged surface region



Schematic sketch of damaged surface region and modeling [1-2]



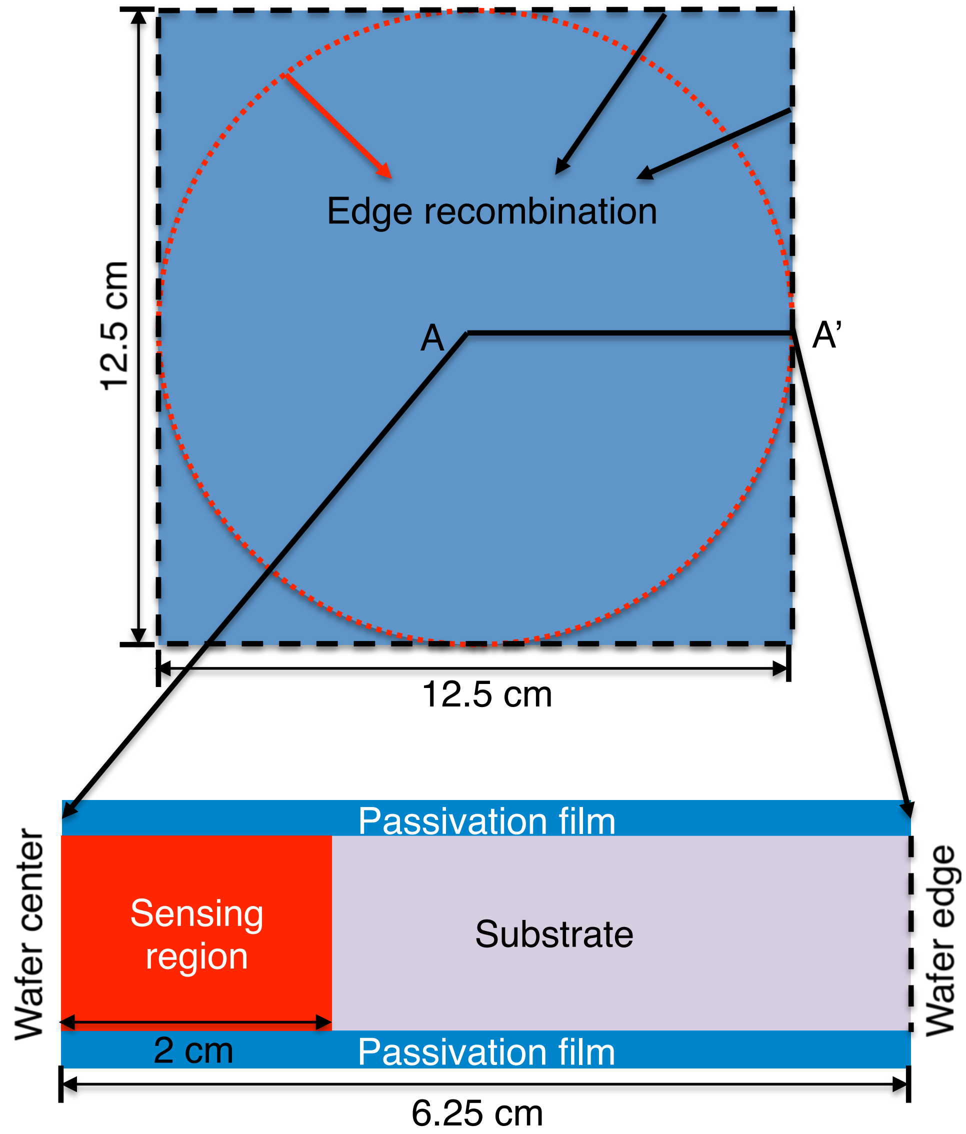
Enhanced SRH recombination in damaged surface region under inversion

[1] I. Martin *et al.*, *23rd EUPVSEC*, pp. 1388-1392, 2008.

[2] S. Steingrube *et al.*, *Phys. Status Solidi RRL,* ***4****,* 91, 2010.

Possible mechanisms – edge recombination

- Edge recombination leads to enhanced recombination [1-2]
- Edge effect is accounted for using a 2D cross section with a cylindrical coordinate



[1] M. Kessler *et al.*, *J. Appl. Phys.*, **111**, 054508, 2012.
[2] B. Veith *et al.*, *Sol. Energy Mater. Sol. Cells,* **120, Part A**, 436, 2014.

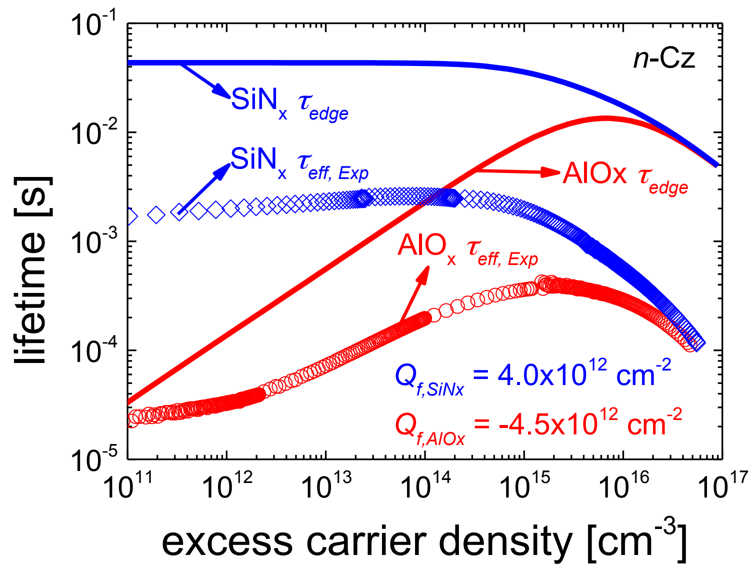
Edge recombination evaluation

- Edge lifetime τ_{edge} is defined as

$$\tau_{edge} = \frac{\Delta n}{\frac{2\pi r W U_{edge}}{\pi r^2 W}} = \frac{\Delta n}{\frac{2U_{edge}}{r}}$$

- r: The radius of the simulation domain
  U_{edge}: The average edge recombination rate

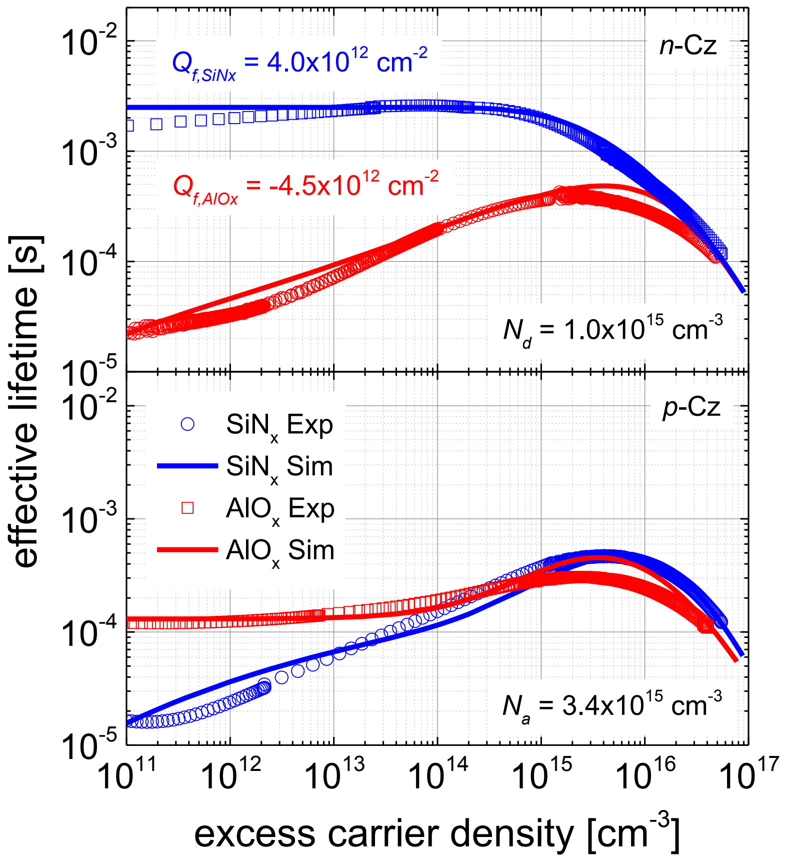
- Edge recombination (worst scenario already): NOT the dominant mechanism for 5 inch and larger



Simulated edge lifetime vs. measured effective lifetime on n-type substrates

Surface damage and edge effect

- Surface damage:
  Very likely as effective lifetime results of both *p*-type and *n*-type lifetime samples were reproduced [1]

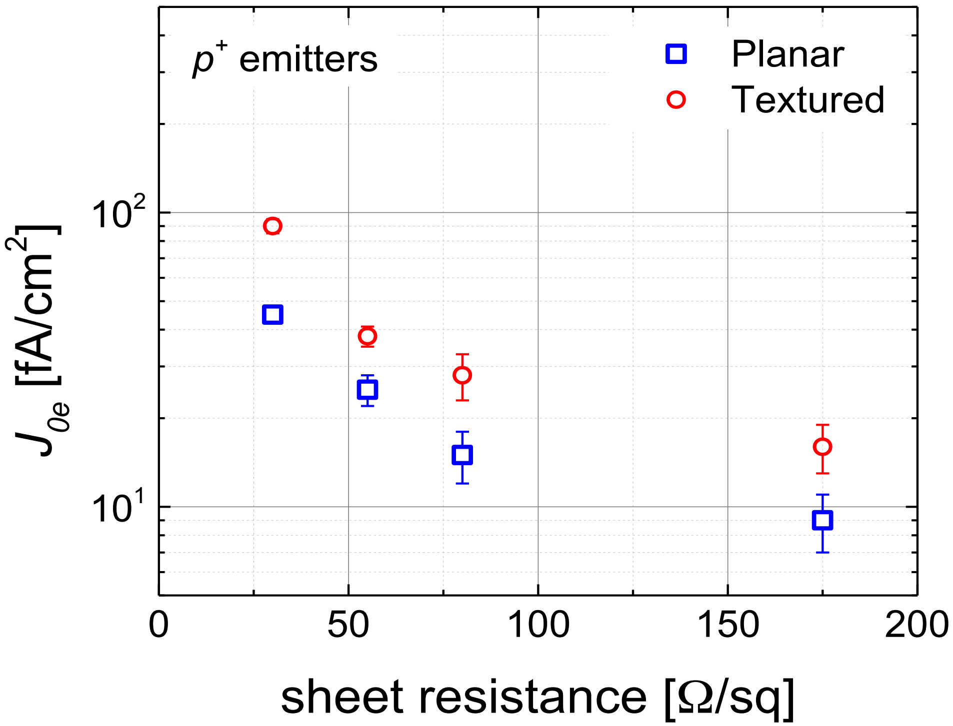


Measured effective lifetime curves are reproduced assuming surface damage

[1] Z. Hameiri and F.-J. MA, *J. App. Phys.*, **117**, 085705, 2015.

Revealing the underlying physics

- ❑ Experimental results may not provide many insights
- ❑ Simulation helps discover the underlying physics

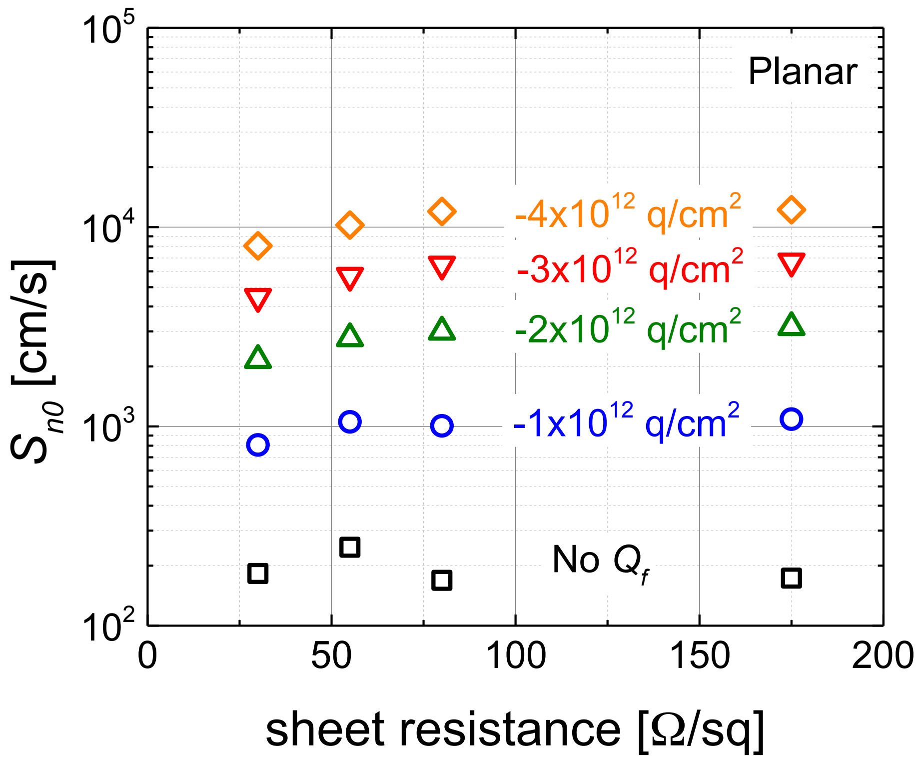


Measured J_{0e} values as a function of boron emitter sheet resistance passivated with PECVD AlO_x/SiN_x dielectric stack [1]

[1] S. Duttagupta *et al.*, *Prog. Photovolt: Res. Appl.*, **21**, 760, 2014.

Example: Chemical passivation analysis of p^+ emitters on planar

- With measured doping profiles and fixed charge density, S_{n0} can be determined for each emitter
- Chemical passivation of AlO on planar surface is independent of sheet resistance and surface doping concentration, same as reference 1
- How about that on a textured surface?



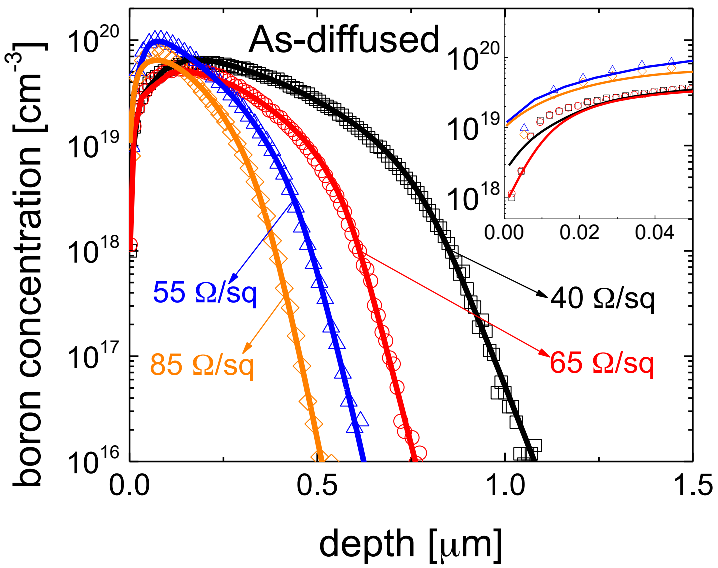
Extracted S_{n0} for various Q_f on planar wafers

[1] L. E. Black *et al.*, *J. App. Phys.*, **115**, 093704, 2014.

Example: Chemical passivation analysis of p^+ emitters on textured

- Surface passivation study on textured wafers can be done by a combination of process and device simulations [1]

- Calibrate diffusion parameters using 1D simulation

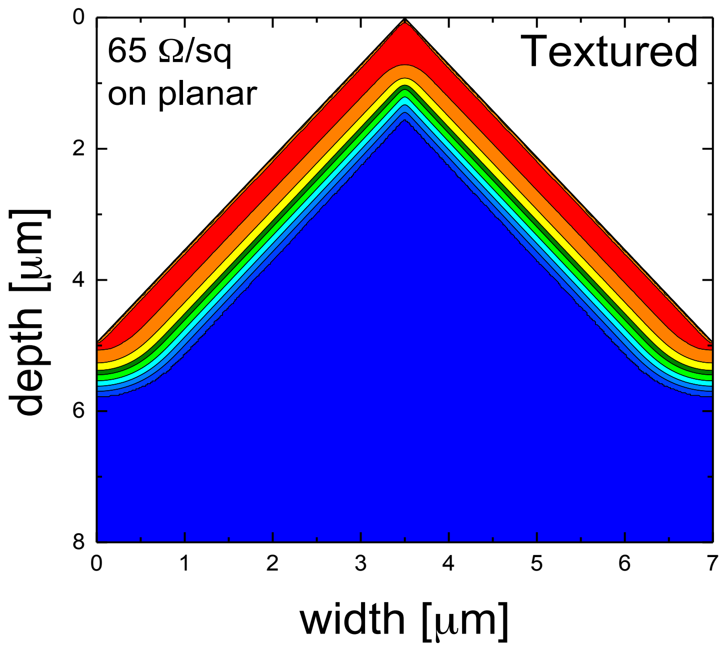


Process simulation was calibrated using 1D SIMS profiles

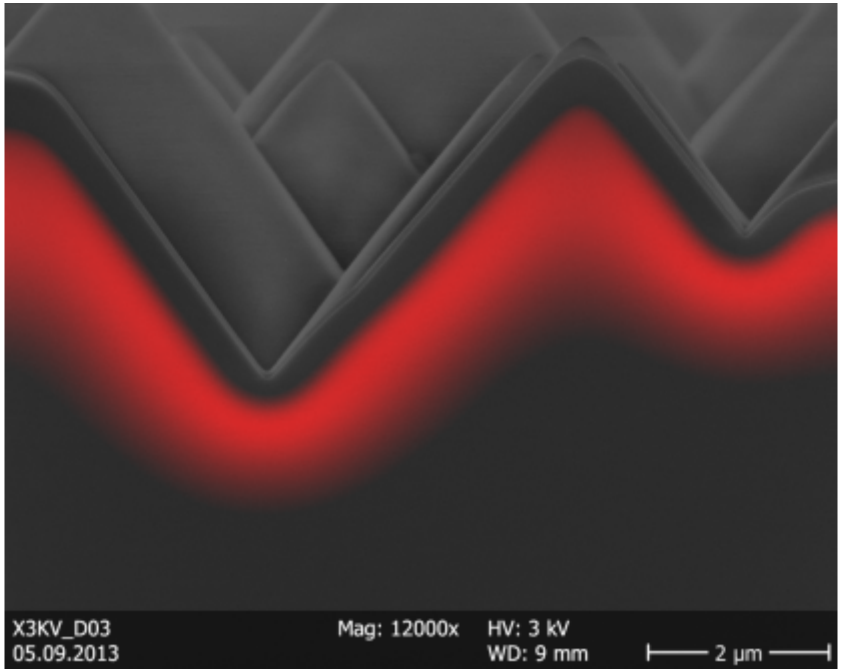
[1] F.-J. Ma *et al.*, *J. App. Phys.*, **116**, 184103, 2014.

Example: Chemical passivation analysis of p^+ emitters on textured

- Simulate boron profiles under the textured surface and verify them against measurement



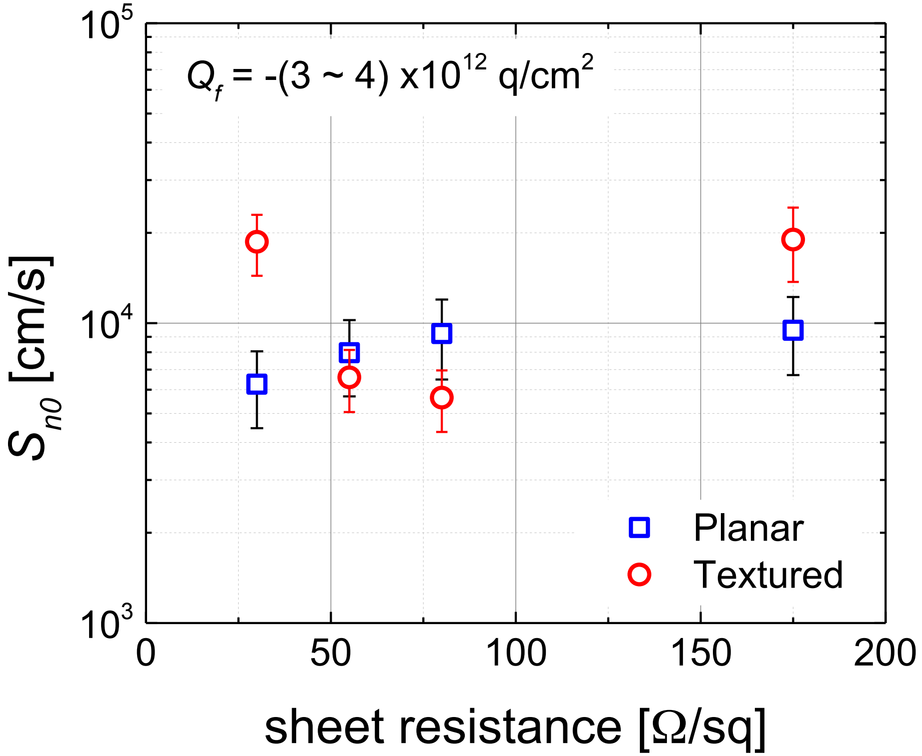
Simulated 65 Ω/sq boron profile under the textured surface



The overlaid SEM and EBIC images of 65 Ω/sq underneath the textured surface

Example: Chemical passivation analysis of p^+ emitters on textured

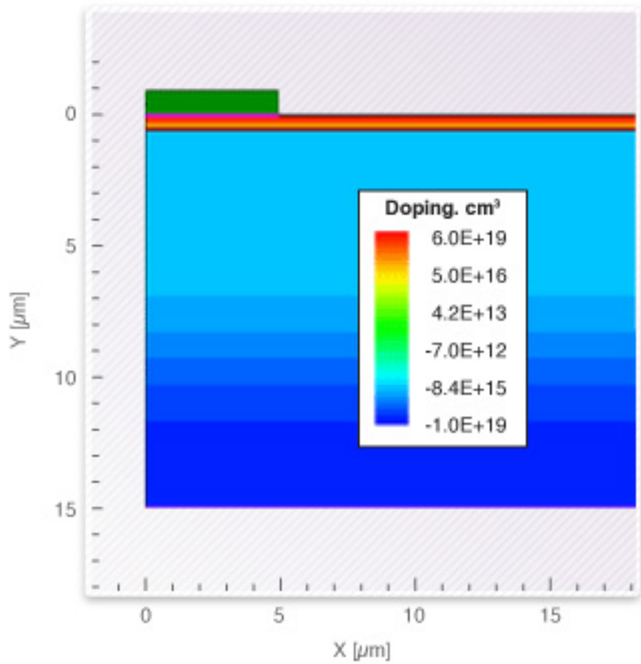
- ❑ Extract S_{n0} for textured samples
- ❑ Chemical passivation of AlO is also independent of surface topology



Extracted S_{n0} on planar and textured wafers for the measured Q_f.

Discovering new phenomena

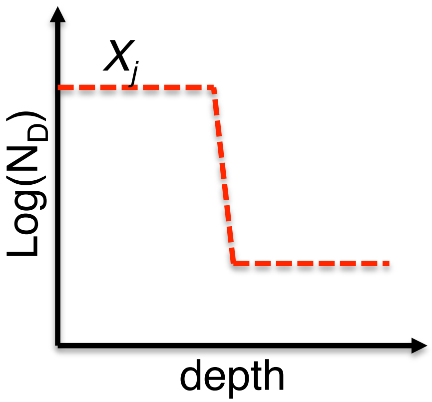
- New phenomena may be discovered by
  - Pushing towards the limits
  - Changing structure
  - Changing the boundaries conditions
  - …



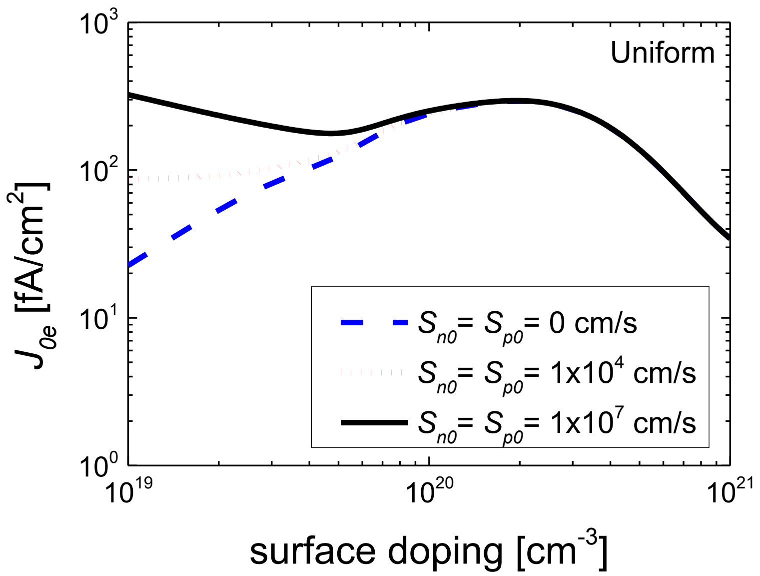
A unit solar cell modeled in TCAD showing the doping distribution

Example: Field effect passivation

- Lower doping concentration is typically desired for emitters
- What if the doping concentration is very high? [1]



Schematic sketch of a uniform phosphorus emitter with a junction depth of 1 µm



Simulated J_{0e} values for phosphorus emitters (X_j = 1 µm)

[1] F.-J. Ma, *PhD thesis*, 2014.

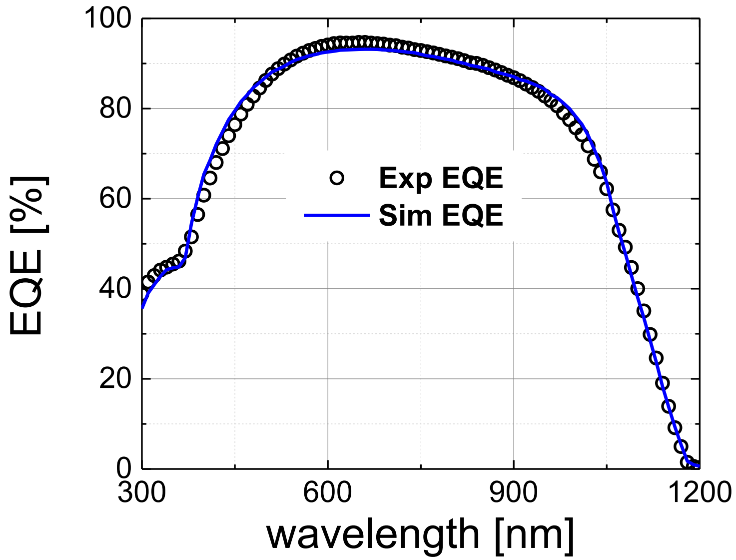
Example: Field effect passivation

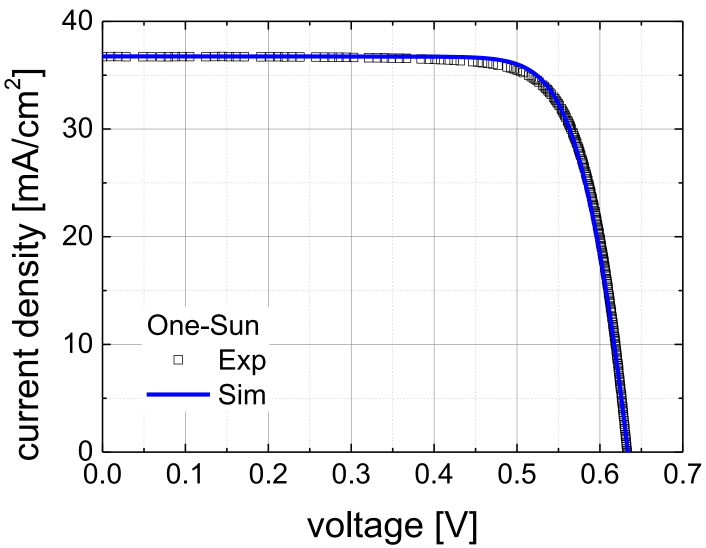
- Possible explanation: Strong field effect from doping suppresses not only surface but also bulk recombination [1]
  - Pros: Doping concentration in the emitter can be adjusted to achieve very low sheet resistance
  - Cons: Bandgap narrowing is strong
- Possible applications: Fingerless solar cell?
- Verification: No

[1] F.-J. Ma, *PhD thesis*, 2014.

Predicting performance improvement

- ❑ A solar cell may be well modelled with reasonable accuracy [1]
- ❑ Performance improvement can be readily predicted
  - ➢ Efficiency
  - ➢ J_{sc}
  - ➢ V_{oc}
  - ➢ FF





[1] F.-J. Ma, *unpublished*, 2014.

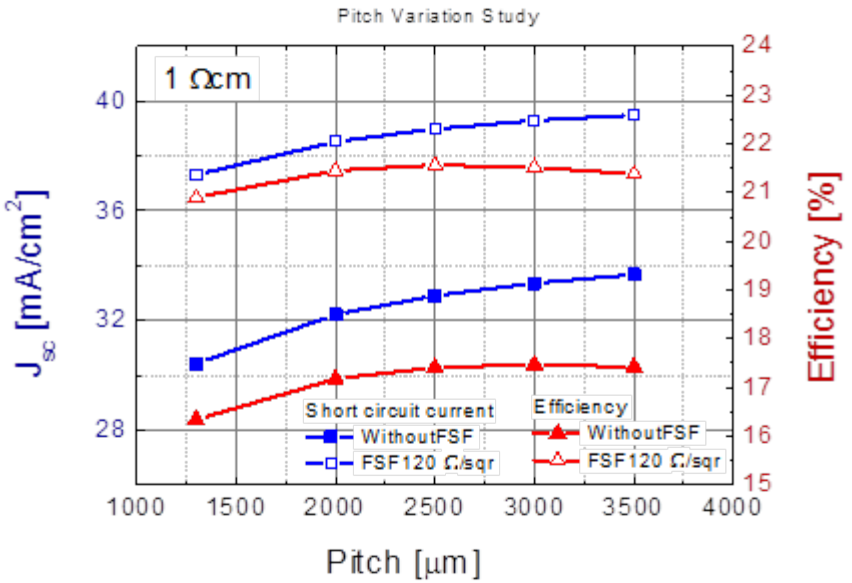
Predicting performance improvement

- Possible improvements based on actions taken on the solar cell

Actions	Efficiency [%]	V_{oc} [mV]	J_{sc} [mA cm^{-2}]	FF [%]
A	18.28	633.0	36.7	78.7
B	18.68	641.8	36.7	79.3
C	18.76	644.5	36.75	79.2
D	18.84	646.7	36.79	79.2

Deterministic modelling

- Deterministic modelling applies to variation studies
  - Process variables
  - Device variables
  - …

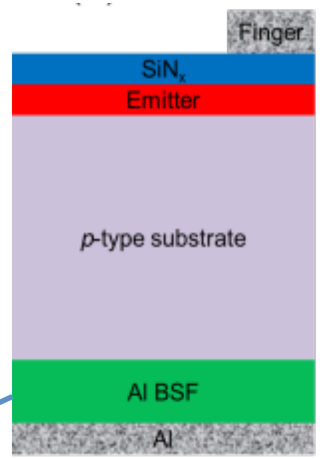


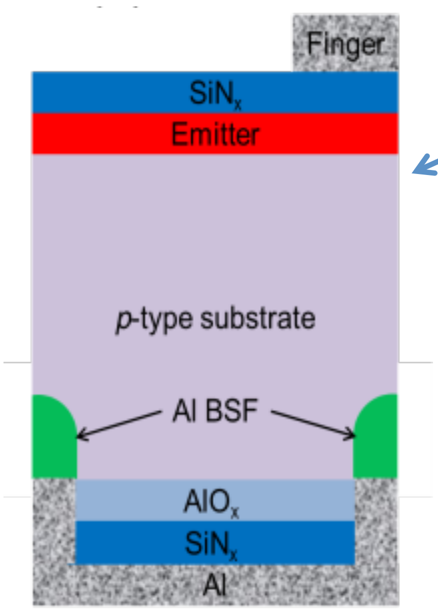
A pitch variation study for an all-back-contact solar cell [1]

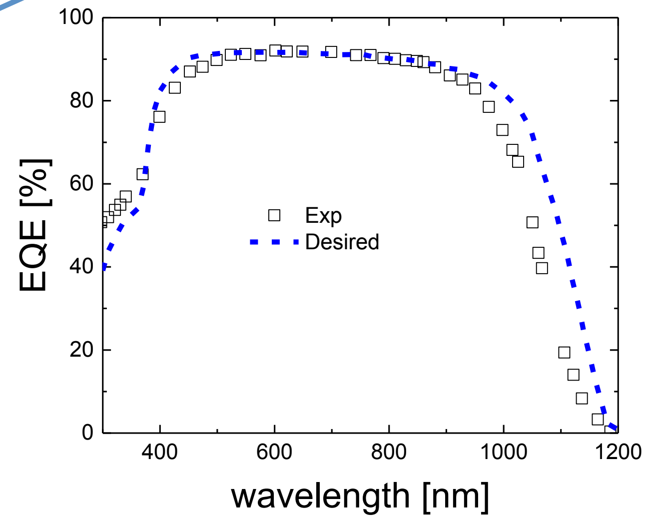
[1] F.-J. Ma, *unpublished*, 2011.

Inverse modelling

- ❑ Typical modelling
  - ➢ Known structure -> known characteristics
- ❑ Inverse modelling
  - ➢ Desired characteristics -> a new structure



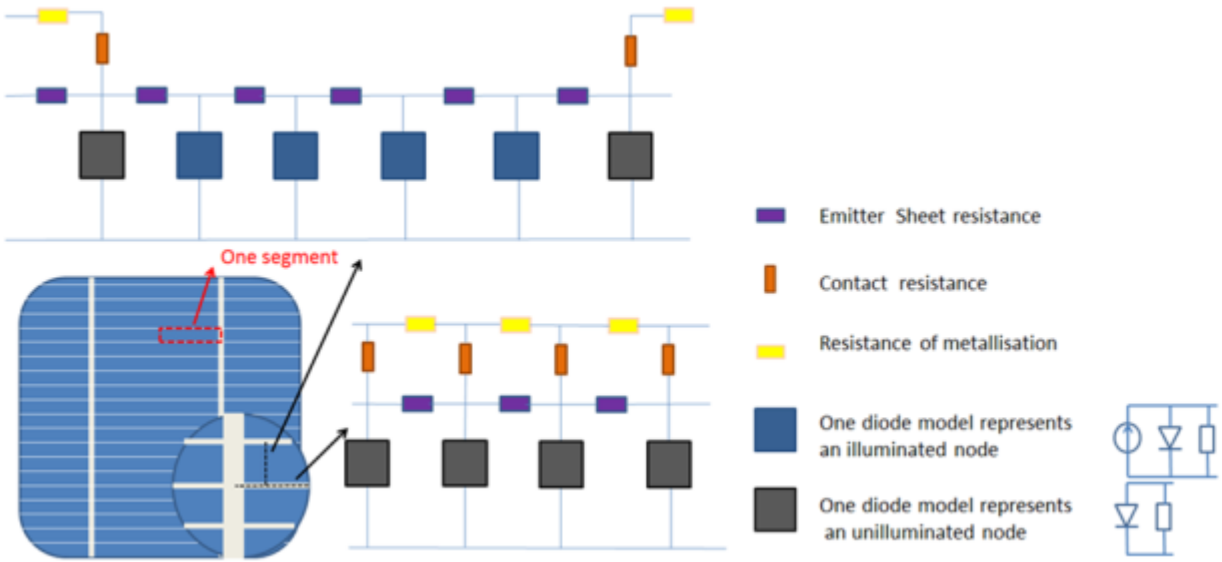




Inverse modelling of a desired EQE curve

Compact modelling

- Feeding TCAD results to circuit design
  - Module simulation
  - Application simulation
  - …



Two intersection of the distributed circuit model in the direction perpendicular (upper) and parallel (right) to fingers, respectively [1]

[1] S. Guo *et al.*, *Energy Procedia*, **25**, 28, 2012.

Summary

- A few benefits of applying TCAD in solar research are highlighted with examples of my previous work
- More benefits can be discovered later with your involvement

Contacts

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- ❑ Thanks to the colleagues and students in SERIS for exciting discussions
- ❑ Thanks to Dr. Ziv HAMEIRI for the fruitful collaboration and the efforts on to bring me here!