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

Speaker: Dr. Fa-Jun MA

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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 many 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
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

Basic equations governing electrical behaviors of semiconductors

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

\[ J_n = q \mu_n n E + q D_n \nabla n = q \mu_n \left( n E + \frac{kT}{q} \nabla n \right) \]

\[ J_p = q \mu_p p E - q D_p \nabla p = q \mu_n \left( p E - \frac{kT}{q} \nabla p \right) \]

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

\[ \frac{\partial p}{\partial t} = G_p - U_p - \frac{1}{q} \nabla J_p \]
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$_2$O$_3$ [1]

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]

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]

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]

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

- Measured injection dependent $\tau_{\text{eff}}$ (passivated by a-SiN$_x$:H) [1]
- Measured injection dependent $\tau_{\text{eff}}$ (passivated by Al$_2$O$_3$) [2]

Example: Field effect surface passivation

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

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.

Edge recombination evaluation

- Edge lifetime $\tau_{\text{edge}}$ is defined as
  \[ \tau_{\text{edge}} = \frac{\Delta n}{\frac{2\pi r W U_{\text{edge}}}{\pi r^2 W}} = \frac{\Delta n}{2 U_{\text{edge}} r} \]

- $r$: The radius of the simulation domain
  $U_{\text{edge}}$: 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]

\[ Q_{f, SiNx} = 4.0 \times 10^{12} \text{ cm}^{-2} \]
\[ Q_{f, AlOx} = -4.5 \times 10^{12} \text{ cm}^{-2} \]
\[ N_d = 1.0 \times 10^{15} \text{ cm}^{-3} \]
\[ N_a = 3.4 \times 10^{15} \text{ cm}^{-3} \]

Measured effective lifetime curves are reproduced assuming surface damage

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 AlOₓ/SiNₓ dielectric stack [1]

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

Example: Chemical passivation analysis of $p^+$ emitters on textured wafers can be done by a combination of process and device simulations [1].

- 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.

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

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

Simulated 65 $\Omega$/sq boron profile under the textured surface

The overlaid SEM and EBIC images of 65 $\Omega$/sq underneath the textured surface
Example: Chemical passivation analysis of $p^+$ emitters on textured samples

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

\[ Q_f = -(3 \sim 4) \times 10^{12} \text{ q/cm}^2 \]

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

Sheet resistance [$\Omega$/sq] vs. $S_{n0}$ [cm/s]
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)

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

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

Predicting performance improvement

Possible improvements based on actions taken on the solar cell

<table>
<thead>
<tr>
<th>Actions</th>
<th>Efficiency [%]</th>
<th>$V_{oc}$ [mV]</th>
<th>$J_{sc}$ [mA cm$^{-2}$]</th>
<th>FF [%]</th>
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<td>D</td>
<td>18.84</td>
<td>646.7</td>
<td>36.79</td>
<td>79.2</td>
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</tbody>
</table>
Deterministic modelling

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

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

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]

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.
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