Simulation of silicon based thin-film solar cells
Contents

Introduction

Physical models & quantum tunneling

Material properties

Modeling of specific thin film solar 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
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Theoretical background

Based on coupled drift-diffusion and Poisson equations

\[-\nabla \cdot \left( \frac{\varepsilon_0 \varepsilon}{q} \nabla V \right) = -n + p + N_D (1 - f_D) - N_A f_A + \sum_j N_{ij} (\delta - f_{ij})\]

\[\nabla \cdot J_n - \sum_j R_{nj} - R_{sp} - R_{st} - R_{au} + G_{opt}(t) = \frac{\partial n}{\partial t} + N_D \frac{\partial f_D}{\partial t},\]

\[\nabla \cdot J_p + \sum_j R_{pj} + R_{sp} + R_{st} + R_{au} - G_{opt}(t) = -\frac{\partial p}{\partial t} + N_A \frac{\partial f_A}{\partial t} .\]

- **Bulk/ surface recombination models.**
- **Bulk/ surface trapping effects.**
Advanced model features

- Optical coating model (with multi-layer optical interference effects).
- 3D ray tracing combined with multiple layer optical coating models. Ray tracing performed over the full solar spectrum.
- Wavelength dependence effects in solar spectrum, bulk material and optical coating.
- Bandgap, mobility and lifetime models for some specific materials.
Model features for a-Si

- Exponential tail states & inter-gap dangling bond (DB) states (Gaussian distribution assumed).

Figure source: Semiconductor for solar cells, H J Moeller, 1993 Artech House, Inc.
Quantum tunneling models

- Tunneling - important for simulating thin-film tandem cells

- Modification of classical & local drift-diffusion transport to include non-local quantum transport/tunneling effects.

- Non-local quantum transport models
  - Intraband tunneling.
  - Interband tunneling (tunneling junction).
  - Mini-band tunneling (superlattice).
  - Non-equilibrium fly-over transport.
  - Non-equilibrium quantum escape.
Integrated quantum drift-diffusion model

- Poisson’s Equation
- Wave Mechanics (Quantization/Tunneling/Multi-band k.p Theory)
- Electron/ Hole Drift-Diffusion Model (Energy transport)

- Potential profile
- Space charge
- Injection current
- Tunneling current correction
Interband tunneling – tunnel junction

- **Application:**
  - Solar cell, VCSEL, bipolar cascade laser, LED.
  - Critical for design of many devices.

- **Numerical issues:**
  - Equivalent carrier local generation has convergence issues.
  - Improved convergence using equivalent mobility which is difficult to estimate.
  - New approach: physically based TJ current across junction implemented within drift-diffusion solver.
Tunneling junction lets e$\leftrightarrow$h non-locally

Numerical challenge: current flow across p-n junction through many mesh points.

Example structure Ref: APL, 71, p3752, (1997)
Simulated I-V: both forward & reverse biased

Remark: careful adjustment of contact resistance is necessary to get a good fit of experimental data.

Negative resistance only appears within rather small range of contact resistance.
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Absorption spectrum

Bandgap 1.7 eV for a-Si:H & 1.1 eV for μc(μC)-Si.

Absorption spectrum Comparison

Triple junction (TJ) tandem cell, $\alpha$-Si PIN (1.72 eV) top junction/ $\alpha$-SiGe PIN (1.5 eV) middle junction/ $\alpha$-SiGe PIN (1.25 eV) bottom junction.
ITO/ZnO material

- ITO could be set as a conductive metal layer or as a semiconductor layer with wide bandgap about 3.6 eV. ITO work function ranges from 4.3 eV to 5.1 eV. If setting ITO as transparent, absorption index $k$ is set zero.

- ZnO set as transparent with index $k$ as zero

Spectrum source: http://www.ioffe.ru/SVA/NSM/nk/Miscellaneous/Gif/ito2.gif
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\( \alpha \)-Si:H PIN solar cells

- Amorphous Si (\( \alpha \)-Si:H) materials: tail states near conduction and valence band edge; two deep level dangling bond states donor-like \( D^+/0 \) & acceptor-like \( D^0/- \).
- Tail states - usually exponential distribution; dangling bond states - Gaussian distribution.
- Density of States (DOS), especially dangling bonds states levels in the band gap can be different depending whether the material is p-, intrinsic or n-type.
- Amorphous Si solar cells made of thin films deposited on substrate like glass.

Two PIN devices: one with \( P^+/I/N^+ \) layer thickness as 0.03 \( \mu \)m/ 0.5 \( \mu \)m/0.01 \( \mu \)m respectively (Ref: G A Swartz, JAP 53 (1) 1982 pp712-719); the other with \( P^+/I/N^+ \) layer thickness as 0.009 \( \mu \)m/ 0.5 \( \mu \)m/ 0.02 \( \mu \)m respectively ("Amorphous and Microcrystalline Silicon Solar Cells, Modeling, Materials and Device Technology", book by R E I Schropp & M Zeman).
α-Si:H PIN modeling results & comparison: I

For P⁺/I/N⁺ device (with layer thickness as 0.03µm/0.5µm/0.01µm respectively in Ref: G A Swartz, JAP 53 (1) 1982 pp712-719).

Deep states associated with α-Si increase the series resistance & lead to more resistive I-V curve with degraded cell efficiency.

<table>
<thead>
<tr>
<th>Experimental</th>
<th>Deep states associated with α-Si increase the series resistance &amp; lead to more resistive I-V curve with degraded cell efficiency.</th>
</tr>
</thead>
</table>

Grid shadowing = 6%
α-Si:H PIN modeling results & comparison: II

For P⁺/ I / N⁺ device (with layer thickness as 0.009µm/ 0.5µm/ 0.02µm respectively in Ref: “Amorphous and Microcrystalline Silicon Solar Cells, Modeling, Materials & Device Technology”, book by R E Schropp & M Zeman).

Deep states associated with a-Si increase the series resistance & lead to more resistive I-V curve with degraded cell efficiency.
Effect of deep trap states

Low efficiency of a-Si solar cell is due to deep traps. Simulations for cells without traps show ideal I-V characteristics.
Microcrystalline Si (µ-Si) PIN/α-Si PIN stacked structure.

The random interfaces similar to the left structure modeled with assumed optical absorption enhancement factor to reflect the light trapping effect.
μ-Si/α-Si PIN tandem cells: bandgap

Bottom cell absorbs both low & high energy photons

Top cell absorbs mainly high energy photons
μ-Si/α-Si PIN tandem cells: optical absorption

- At low photon energy region (large wavelength), absorption occurs mainly in the bottom subcell.
- At high photon energy region (low wavelength), absorption occurs in both the bottom and top subcells.
\(\mu\text{-Si}/\alpha\text{-Si}\) PIN tandem cells: comparison of I-V curves

With light tapping optical absorption enhancement, cell efficiency is comparable to the experimental for similar cells.
μ-Si/α-Si PIN tandem cells: I-V curve

Assuming no light trapping; ITO defined as semiconductor; Tunneling implemented between μ-Si & ITO.

Efficiency high up to 11.13%.

Tunneling implemented between top & bottom subcells, also between μ-Si & ITO; Modeling shows higher efficiency.
α-Si/α-SiGe/α-SiGe TJ tandem cell

<table>
<thead>
<tr>
<th>ITO</th>
<th>p_3</th>
</tr>
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<tbody>
<tr>
<td>i_3 a-Si alloy</td>
<td>n_3</td>
</tr>
<tr>
<td>p_2</td>
<td>i_2 a-SiGe alloy</td>
</tr>
<tr>
<td>n_2</td>
<td>i_1 a-SiGe alloy</td>
</tr>
<tr>
<td>p_1</td>
<td>Zinc Oxide</td>
</tr>
<tr>
<td>n_1</td>
<td>Silver</td>
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</tbody>
</table>

- Triple junction (TJ) tandem cell, α-Si PIN (1.72 eV) top junction/ α-SiGe PIN (1.5 eV) middle junction/ α-SiGe PIN (1.25 eV) bottom junction.
Energy band: $\alpha$-Si/$\alpha$-SiGe/$\alpha$-SiGe TJ cell

At bias voltage = 2.9 V
Optic generation: $\alpha$-Si/$\alpha$-SiGe/$\alpha$-SiGe TJ cell

- Top junction - thinnest, bottom junction - thickest
- As top & middle junctions absorb high-energy photons & bottom junction absorbs rest of the high-energy photons & low-energy photons.
I-V curve: $\alpha$-Si/$\alpha$-SiGe/$\alpha$-SiGe TJ cell

Flat layer interfaces assumed. Random texture for light trapping can be handled by FDTD method.

$I_{sc}$: 56.60 A/m$^2$
$V_{oc}$: 2.47 V
Efficiency: 12.03%
Spectrum: AM1.5 Global
Summary

Physical models & quantum tunneling are introduced for Crosslight APSYS together with other advanced modeling features.

Model for a-Si & material absorption properties for a-Si, muC-Si, a-SiGe & ITO/ ZnO described.

Modeling results for a-Si PIN solar cell, dual junction muC-Si/ a-Si & triple junction a-Si/ a-SiGe/ a-SiGe tandem cells are demonstrated.

When combined with Crosslight’s 2D/ 3D ray tracing & FDTD modules, Crosslight APSYS can be effectively utilized for Si-based thin film solar cell design.