Simulation of silicon based thin-film solar cells

CROSSLIGHT
Software Inc.

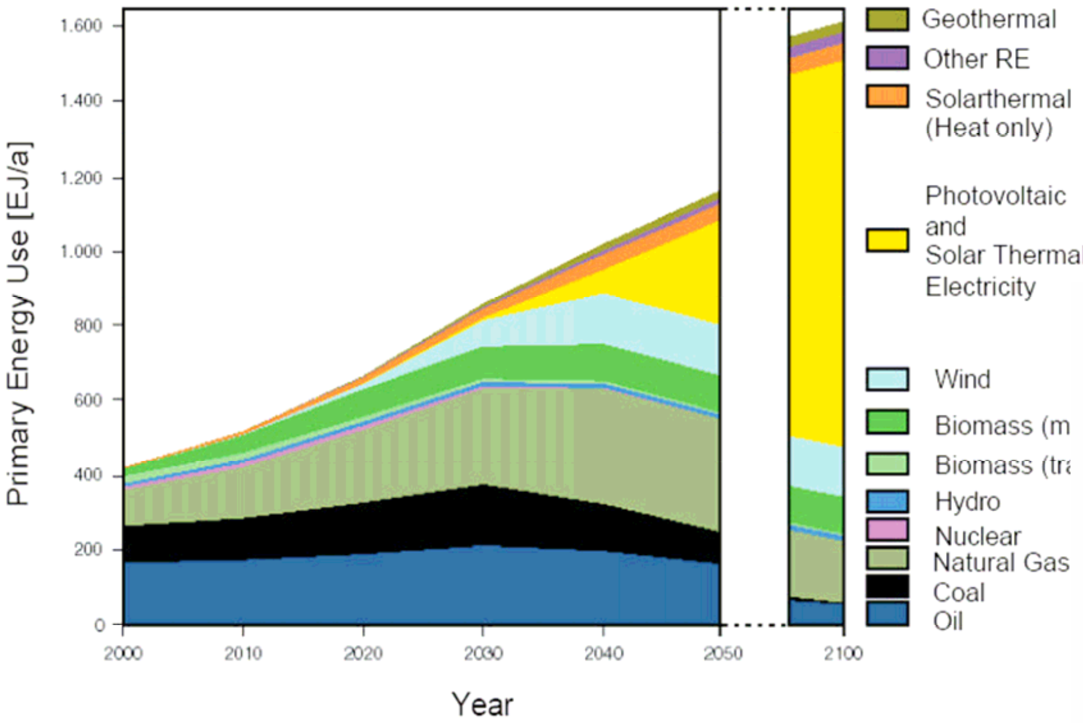
www.crosslight.com

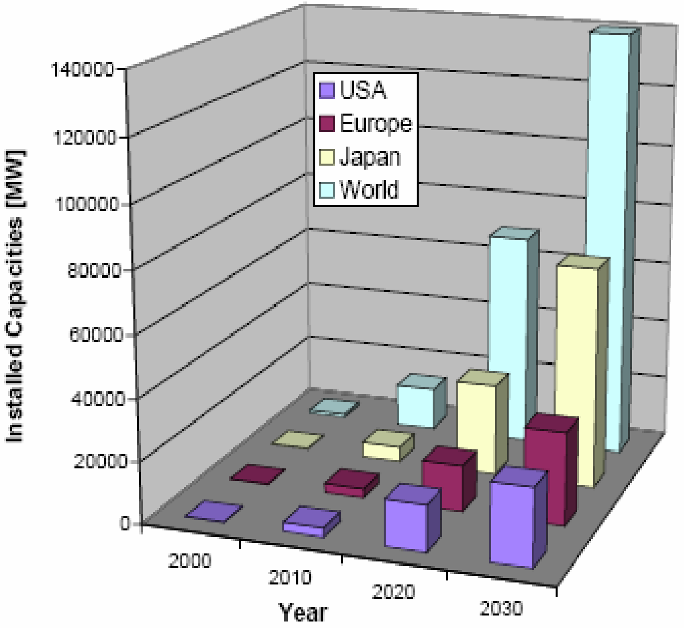
Contents

- ☛ **Introduction**
- ☛ **Physical models & quantum tunneling**
- ☛ **Material properties**
- ☛ **Modeling of specific thin film solar cells**
- ☛ **Summary**

Hot market

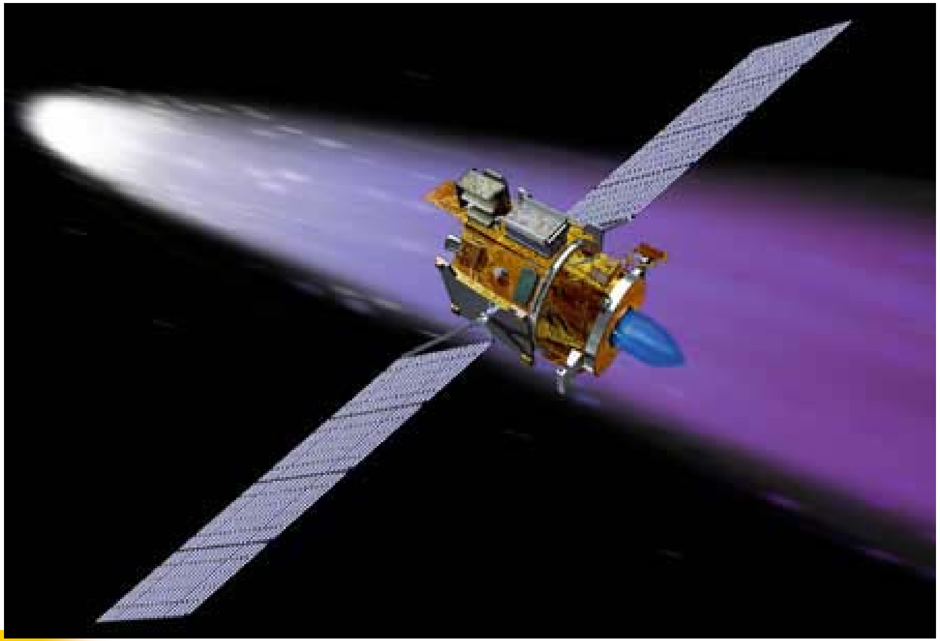
- **Increasing growth of global-wide market for photovoltaic system**





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**

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

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

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

- **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).**

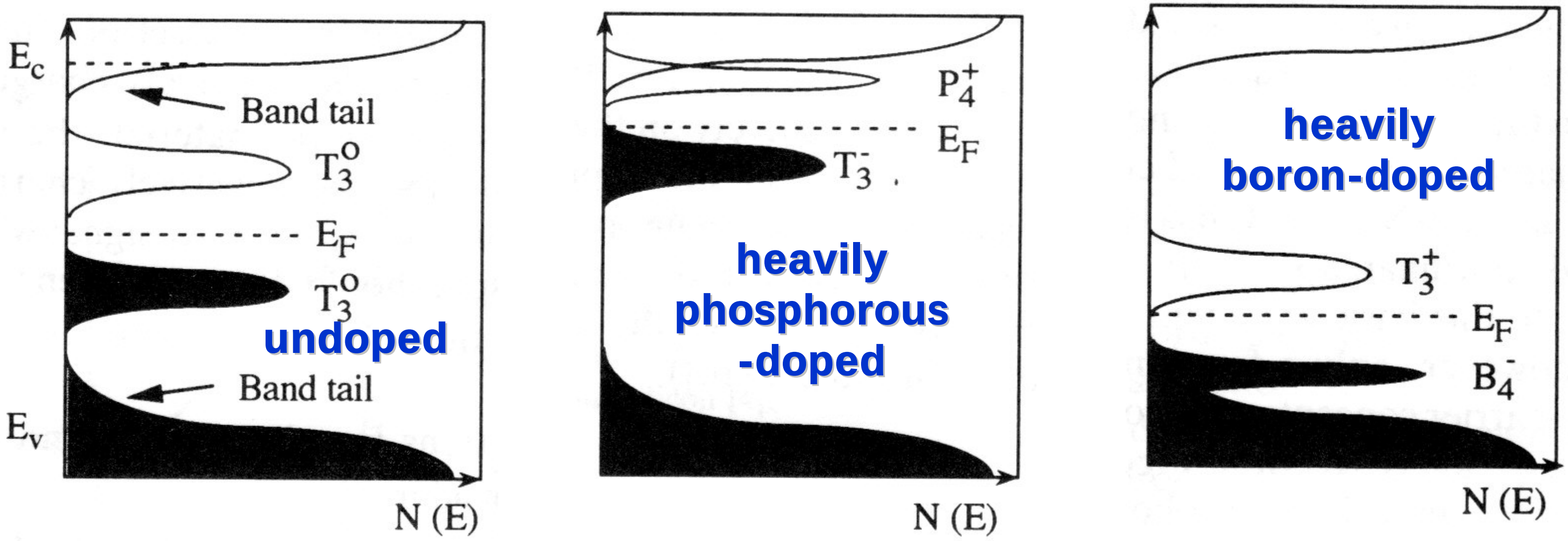
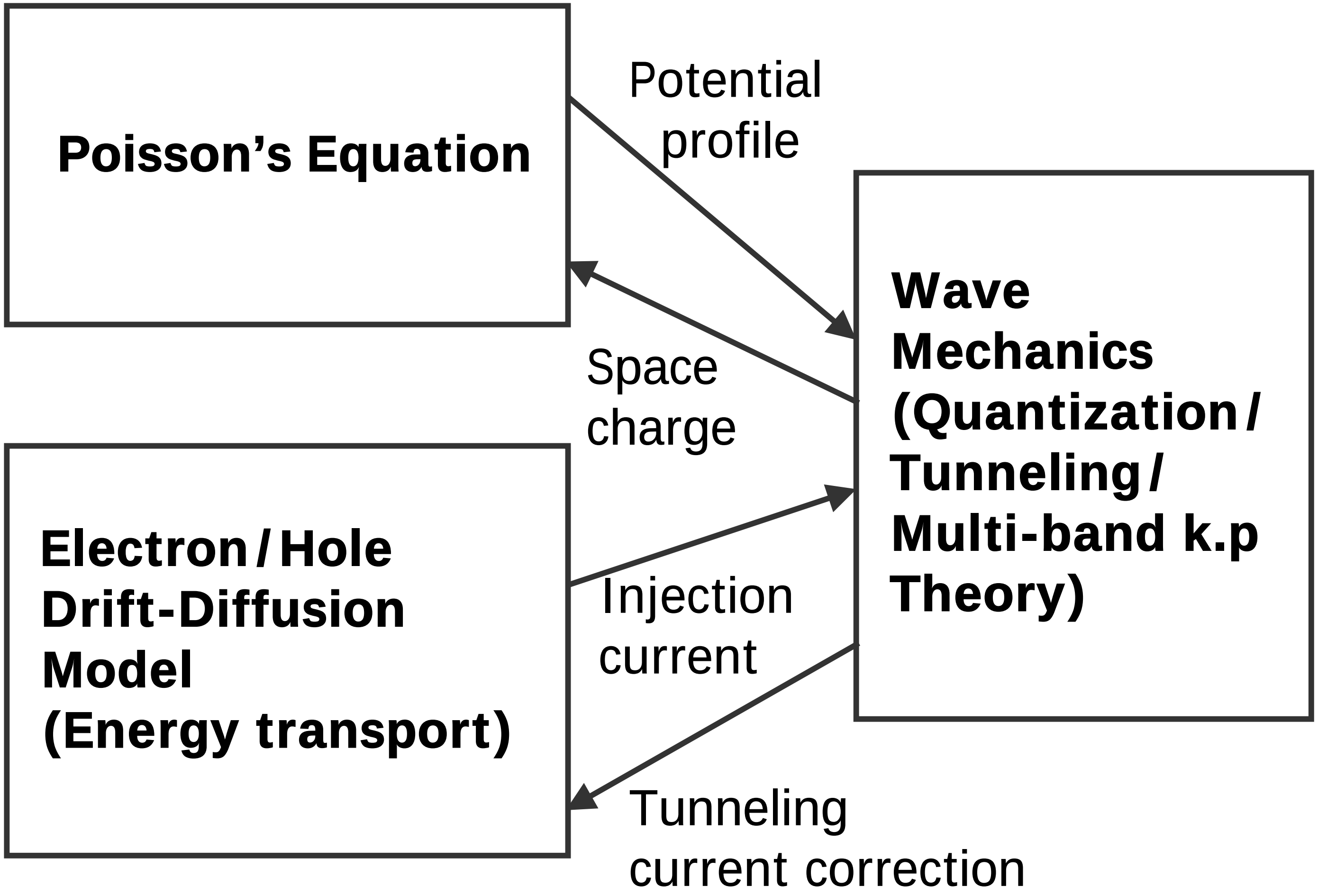


Figure source: Semiconductor for solar cells, H J Moeller, 1993 Artech House, Inc.

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

Potential profile

Space charge

Wave Mechanics (Quantization / Tunneling / Multi-band k.p Theory)

Electron / Hole Drift-Diffusion Model (Energy transport)

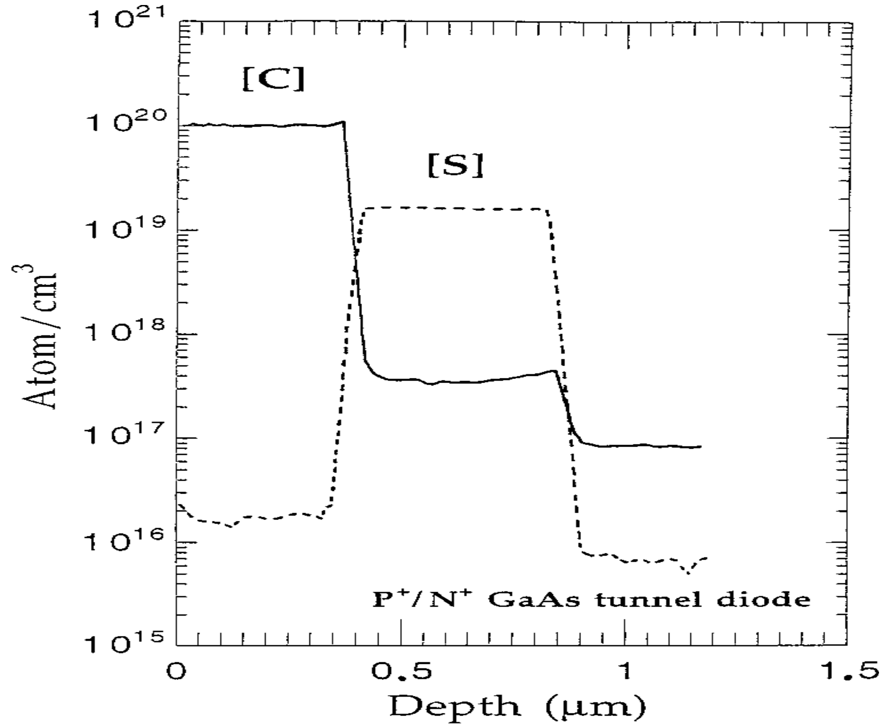
Injection current

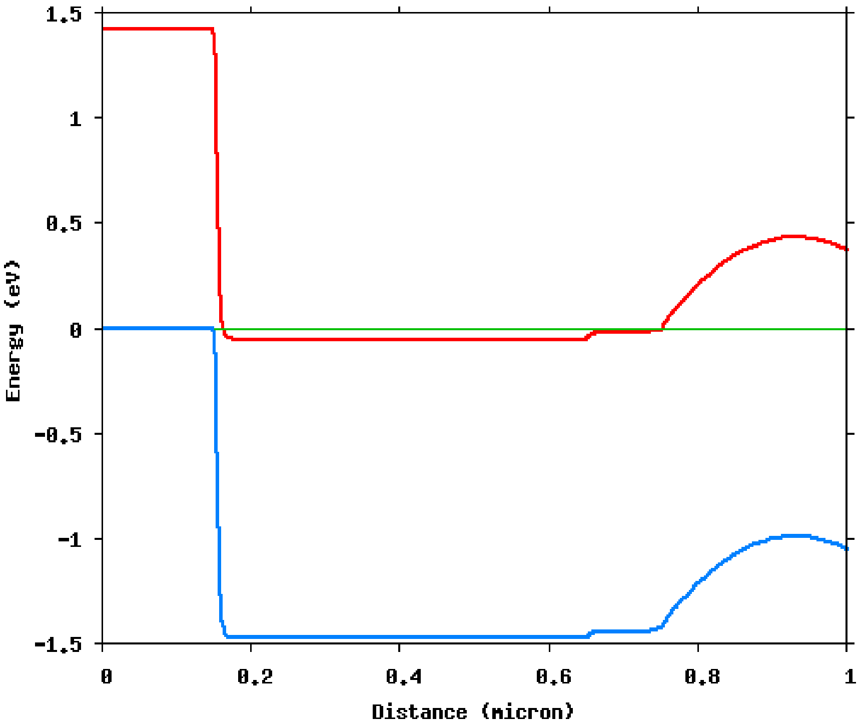
Tunneling current correction

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<-->h non-locally

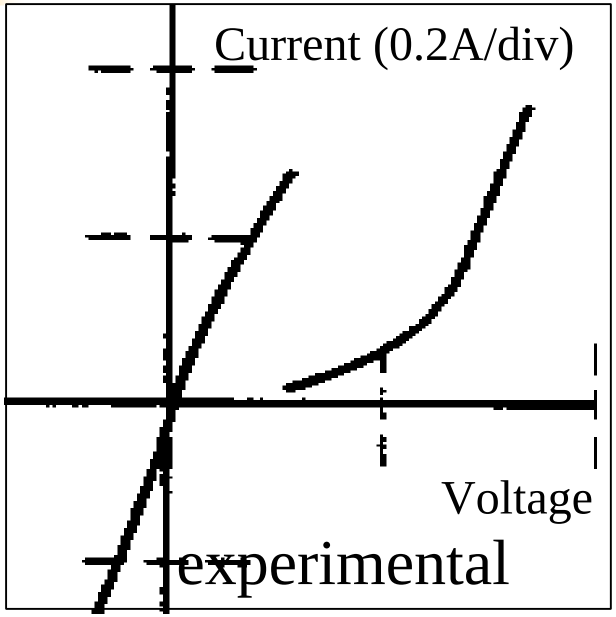


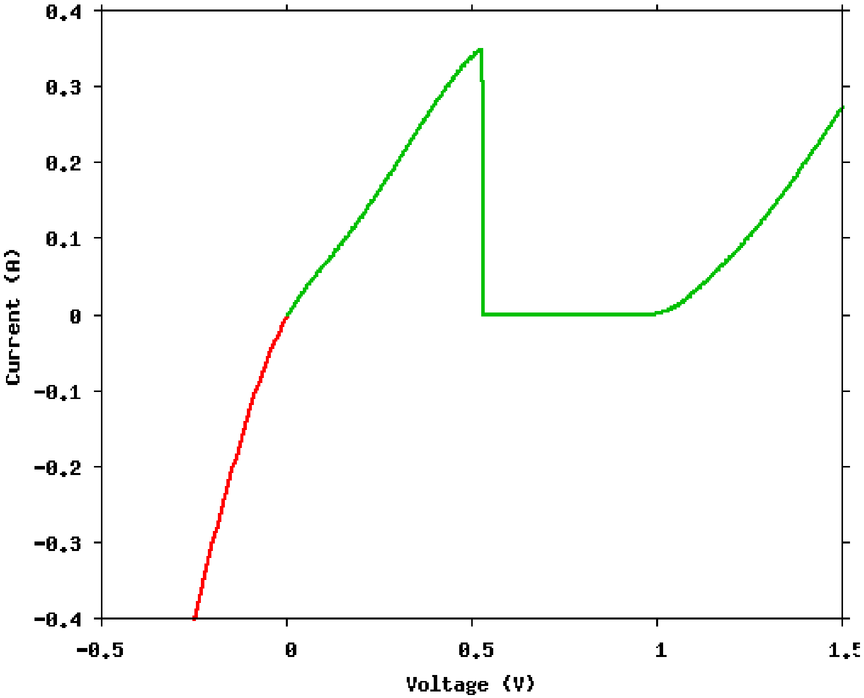


Numerical challenge: current flow across p-n junction through many mesh points.

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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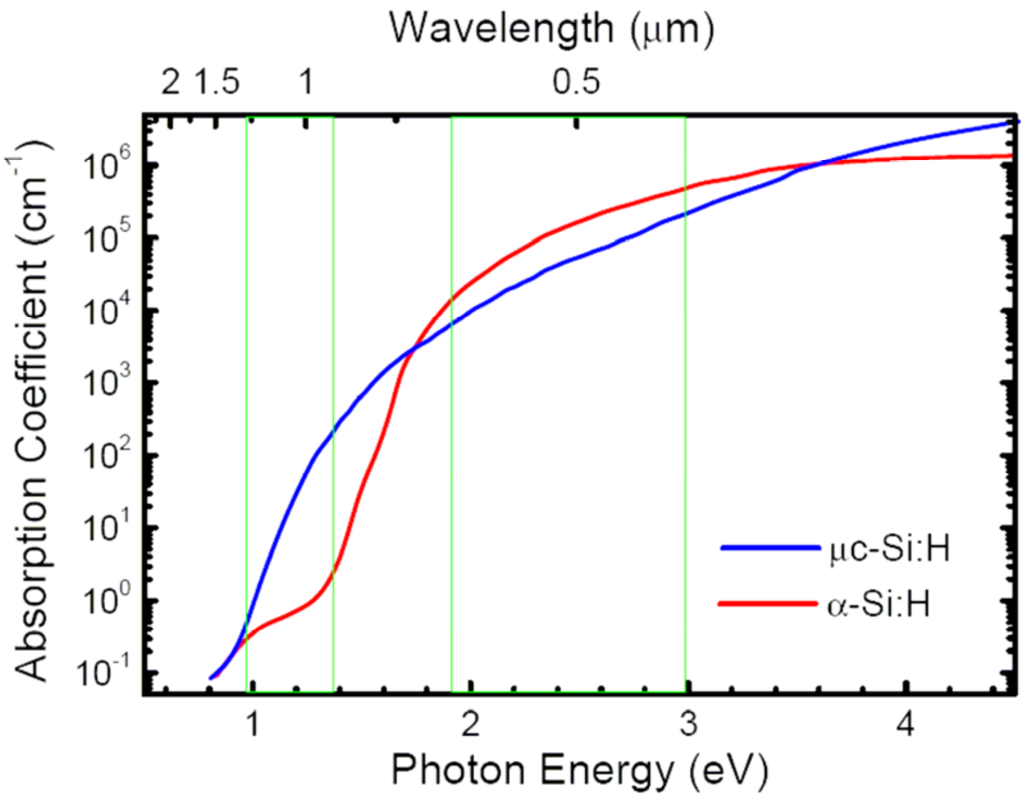
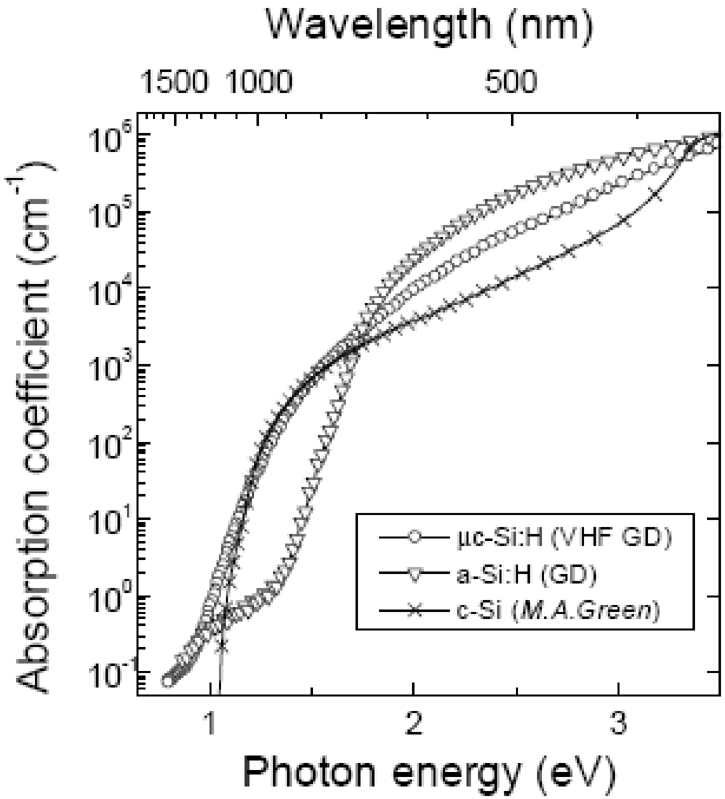
Absorption spectrum

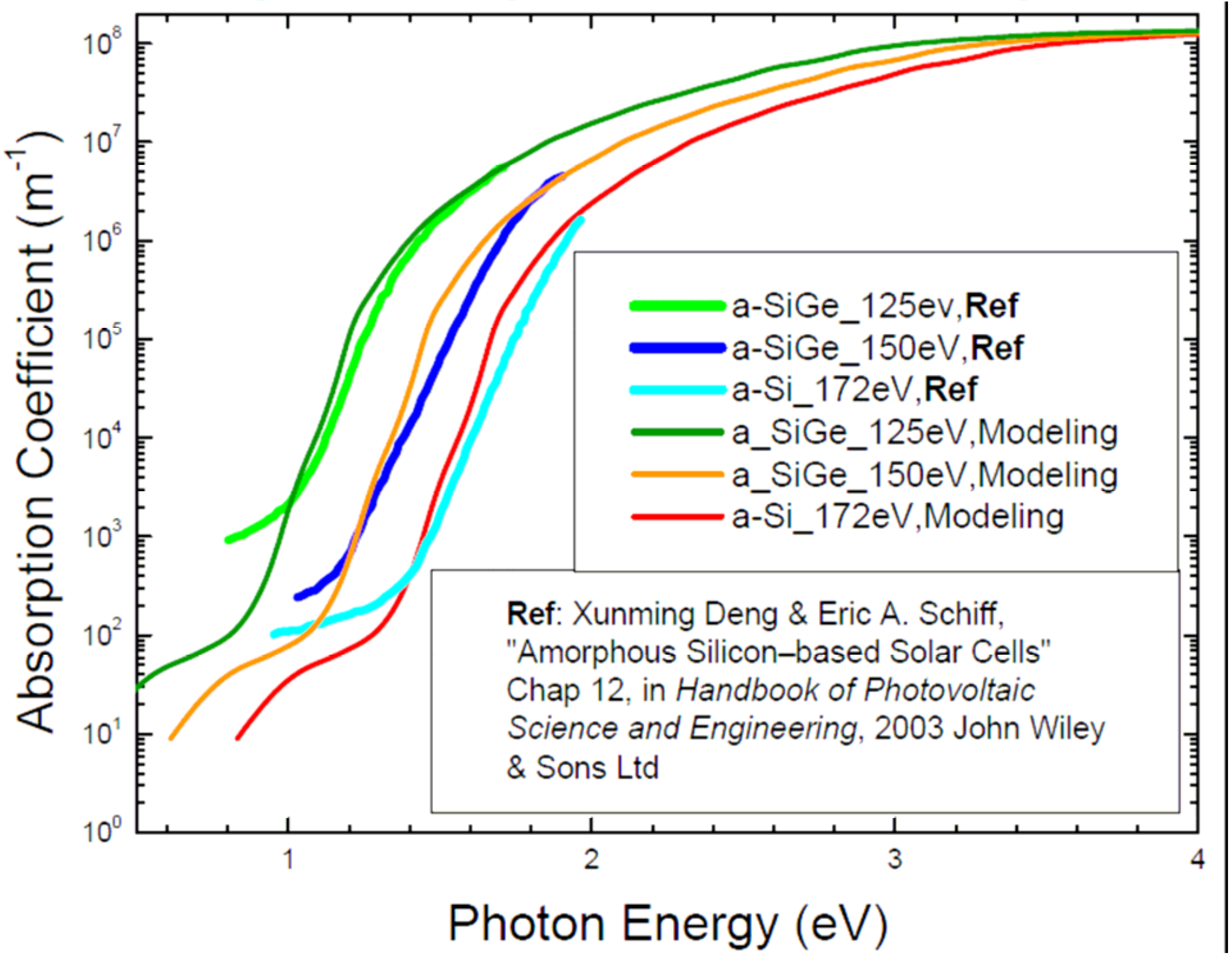
- **Bandgap 1.7 eV for a-Si:H & 1.1 eV for muC(μC)-Si.**





Spectrum source: J. Springer et al, Proc. 16th European Photovoltaic Solar Energy Conference, James&James Sci. Publ. (2000), p. 434.

Absorption spectrum Comparison

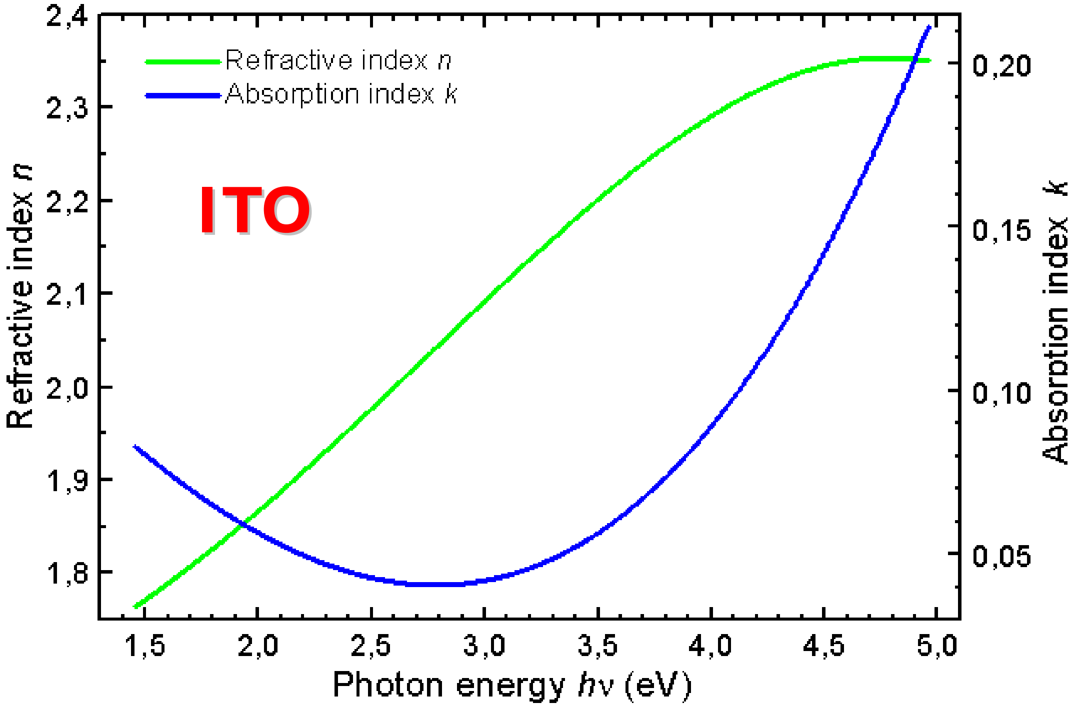


Ref: Xunming Deng & Eric A. Schiff, "Amorphous Silicon–based Solar Cells" Chap 12, in *Handbook of Photovoltaic Science and Engineering*, 2003 John Wiley & Sons Ltd

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.

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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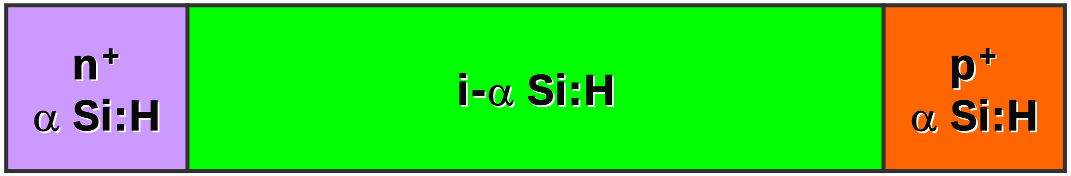
α-Si:H PIN solar cells

- **Amorphous Si (α-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.**

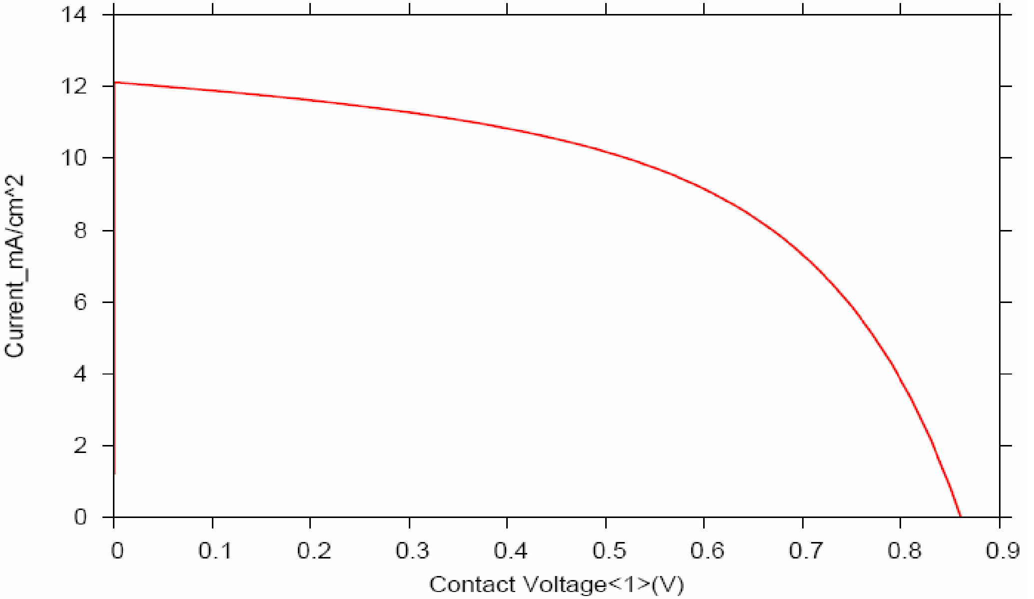


- **Two PIN devices: one with $P^+/I/N^+$ layer thickness as 0.03μm / 0.5μm / 0.01μm respectively (Ref: G A Swartz, JAP 53 (1) 1982 pp712-719); the other with $P^+/I/N^+$ layer thickness as 0.009μm / 0.5μm / 0.02μm respectively ("Amorphous and Microcrystalline Silicon Solar Cells, Modeling, Materials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

α-Si:H PIN modeling results & comparison: I

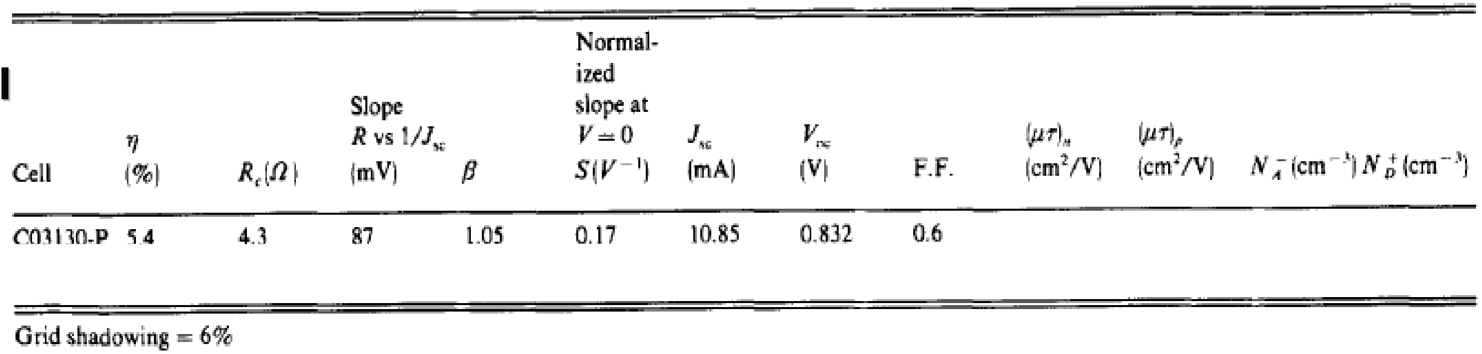
- **For $P^+ / I / N^+$ device** (with layer thickness as 0.03μm / 0.5μm / 0.01μm respectively in Ref: G A Swartz, JAP 53 (1) 1982 pp712-719).

Modeling



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

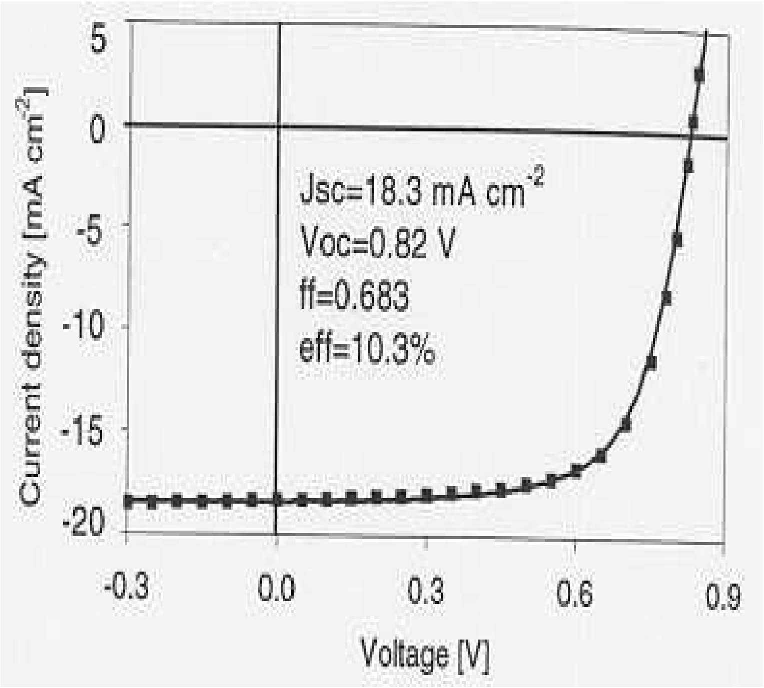
Experimental

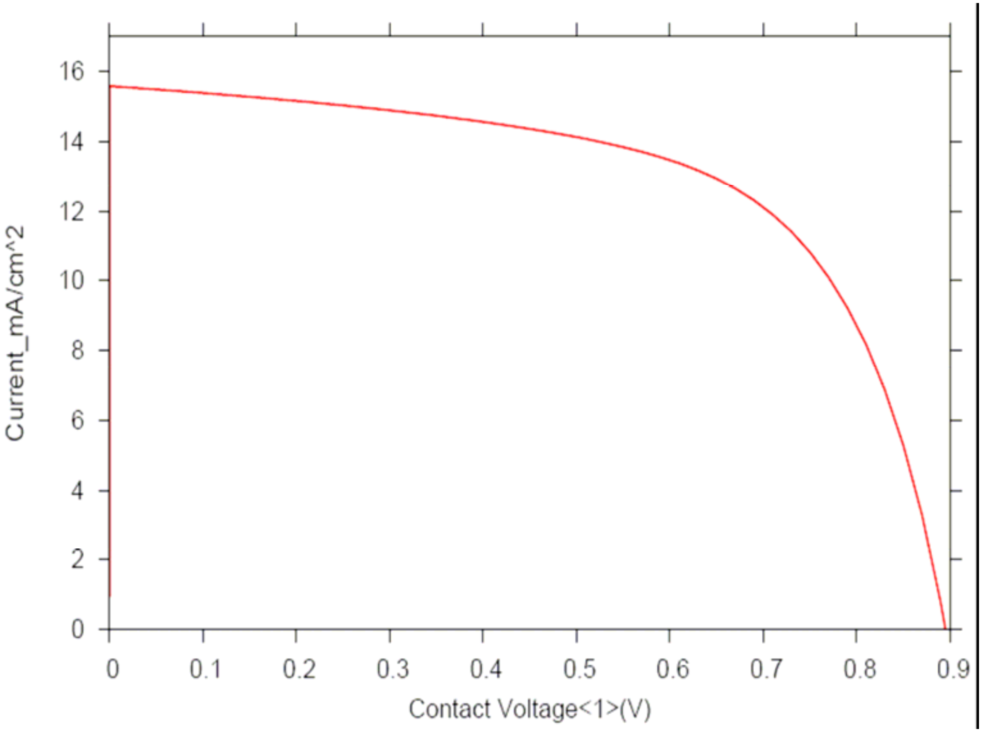


Cell	η (%)	$R_c (\Omega)$	Slope R vs $1/J_{sc}$ (mV)	β	Normalized slope at $V=0$ $S(V^{-1})$	J_{sc} (mA)	V_{oc} (V)	F.F.	$(\mu\tau)_n$ (cm^2/V)	$(\mu\tau)_p$ (cm^2/V)	N_A^- (cm^{-3})	N_D^+ (cm^{-3})
C03130-P	5.4	4.3	87	1.05	0.17	10.85	0.832	0.6				

Grid shadowing = 6%

α-Si:H PIN modeling results & comparison: II



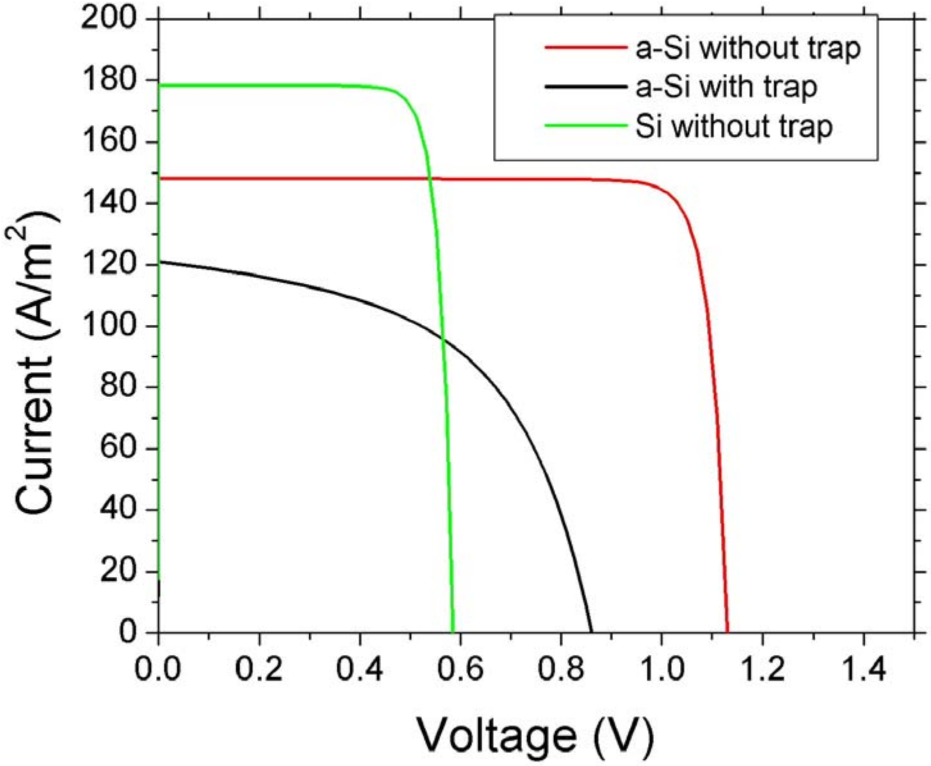


Experimental

Modeling

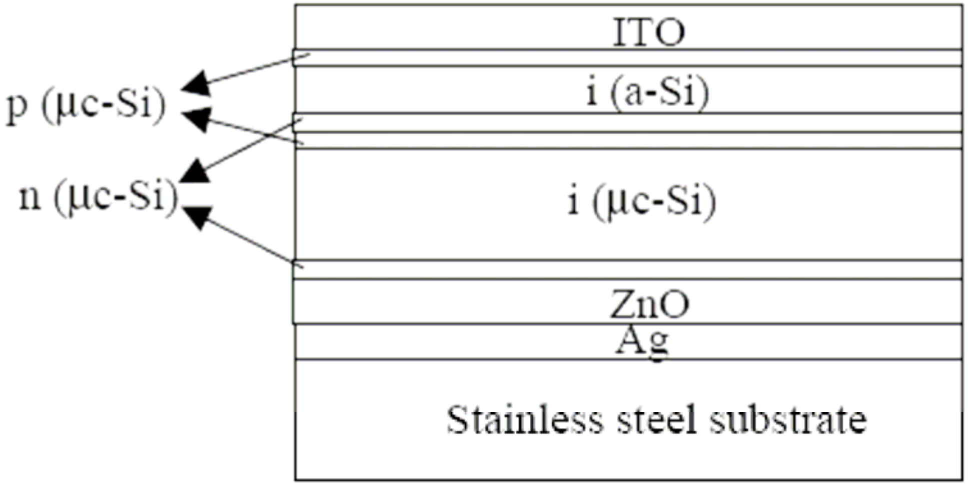
- **For P^+ / I / N^+ device (with layer thickness as 0.009μm / 0.5μm / 0.02μm respectively in Ref: "Amorphous and Microcrystalline Silicon Solar Cells, Modeling, Materials & Device Technology", book by R E Schropp & M Zeman).**
  - **Deep states associated with a-Si increase the series resistance & lead to more resistive I-V curve with degraded cell efficiency.**

Effect of deep trap states

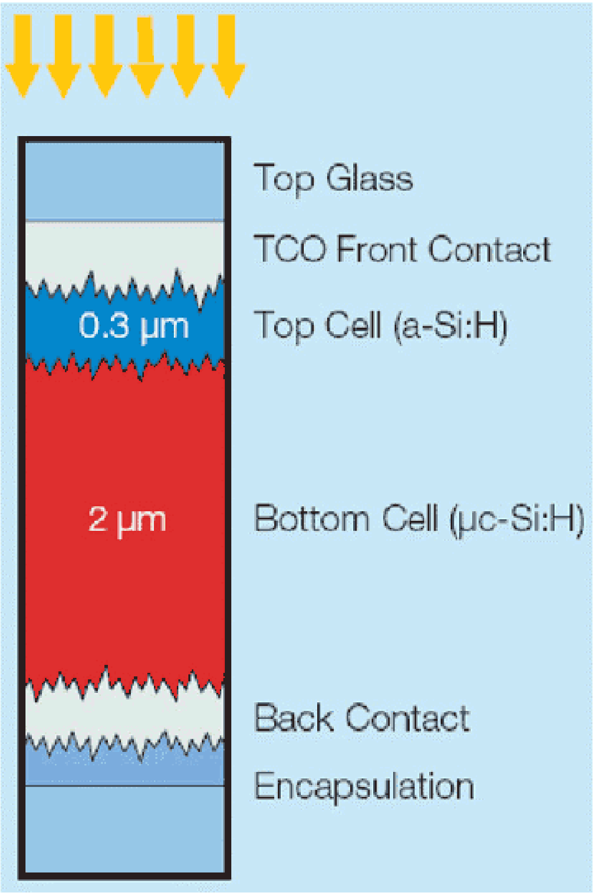


- **Low efficiency of a-Si solar cell is due to deep traps. Simulations for cells without traps show ideal I-V characteristics.**

μ-Si/α-Si PIN tandem cells

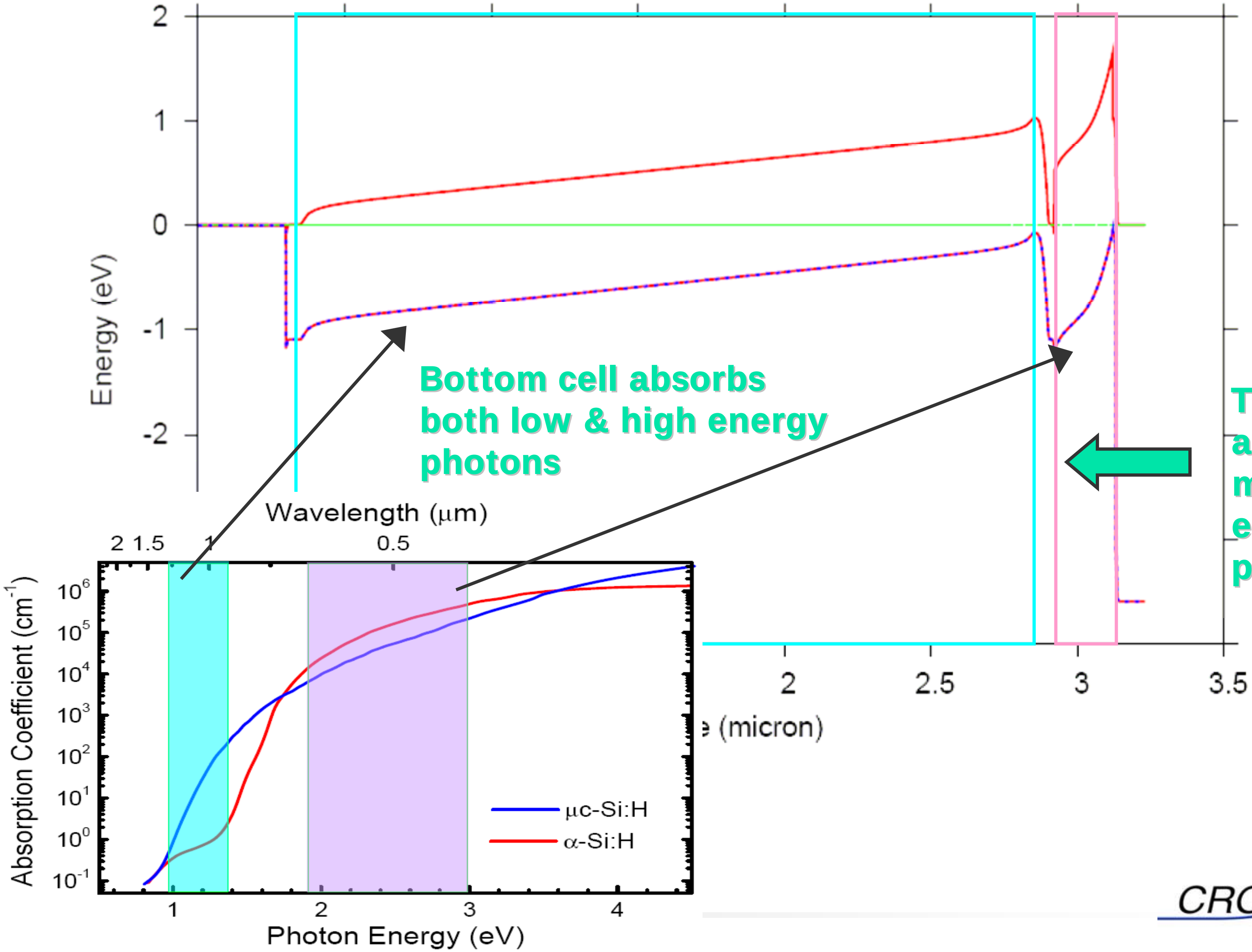


Structure similar to Applied Physics A, vol. 69, p. 169 (1999)



- **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.**

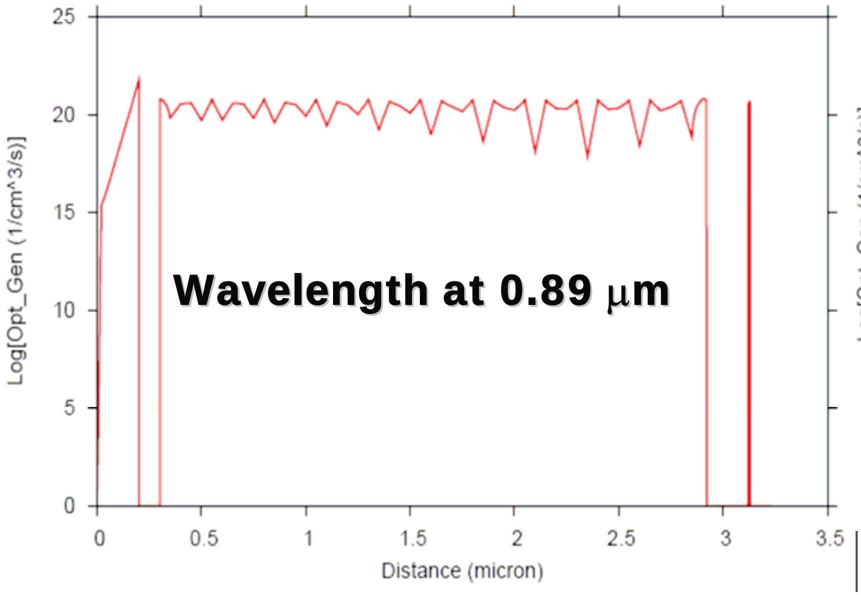
μ-Si/α-Si PIN tandem cells: bandgap

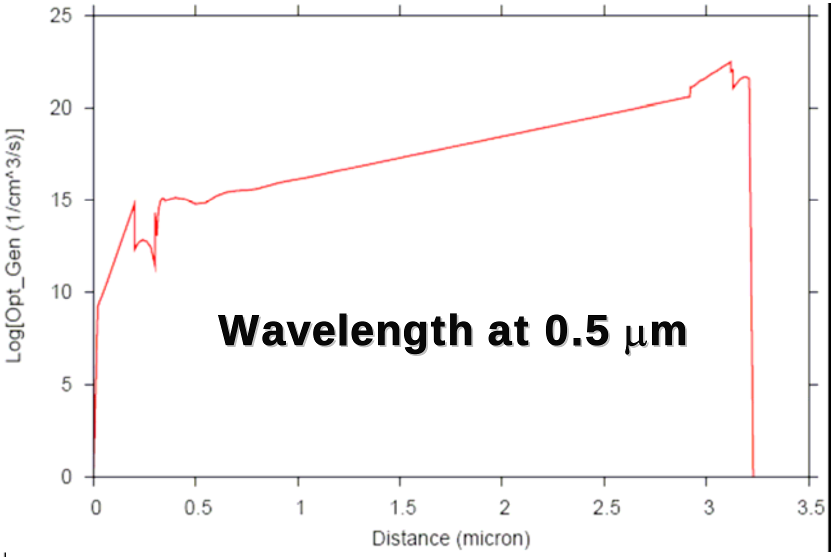


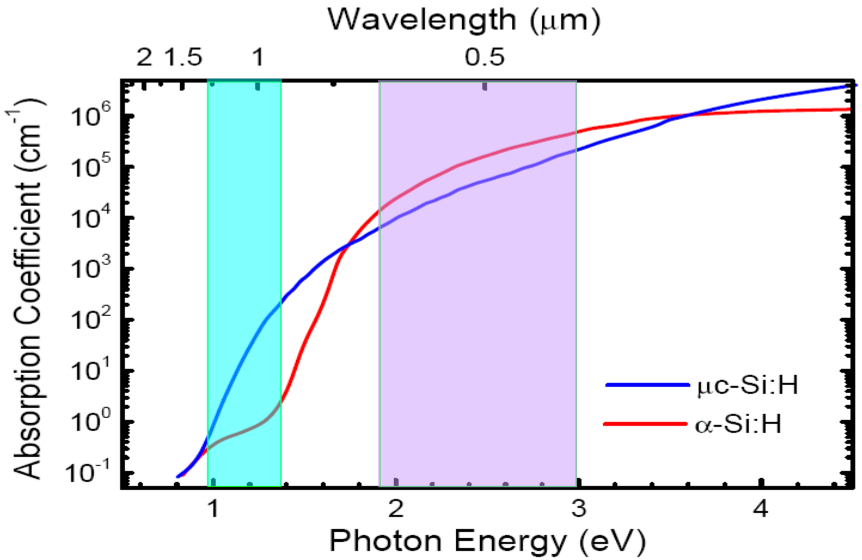
Bottom cell absorbs both low & high energy photons

Top cell absorbs mainly high energy photons

µ-Si/α-Si PIN tandem cells: optical absorption

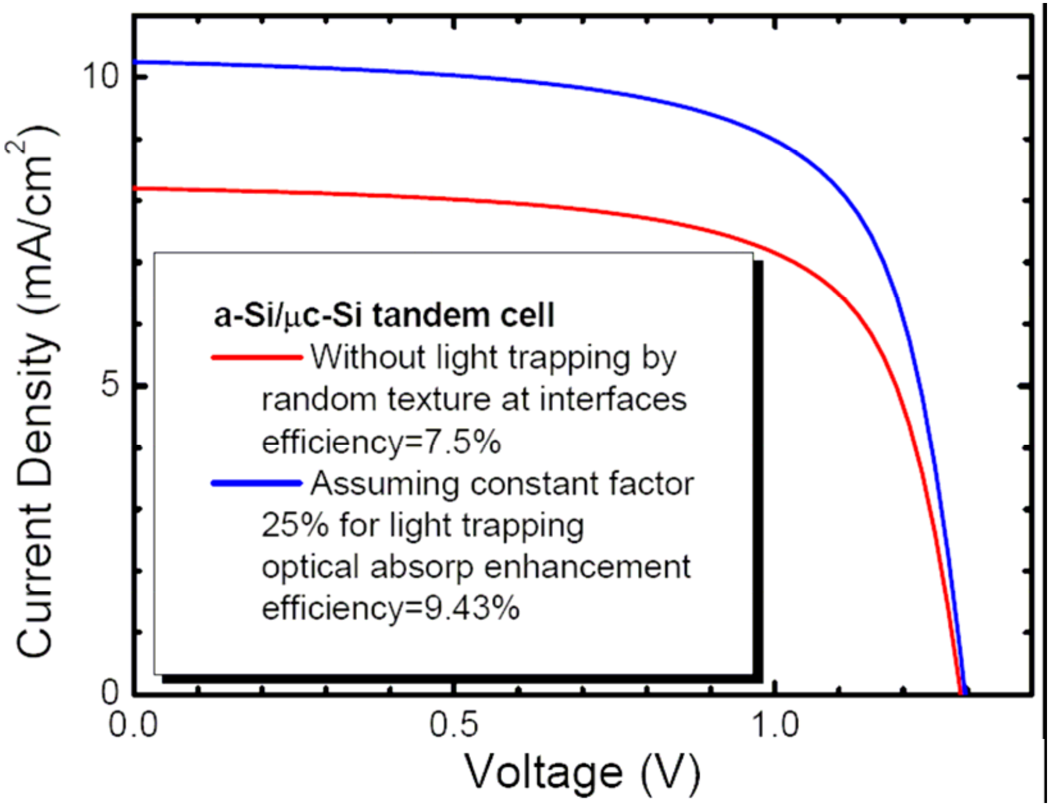






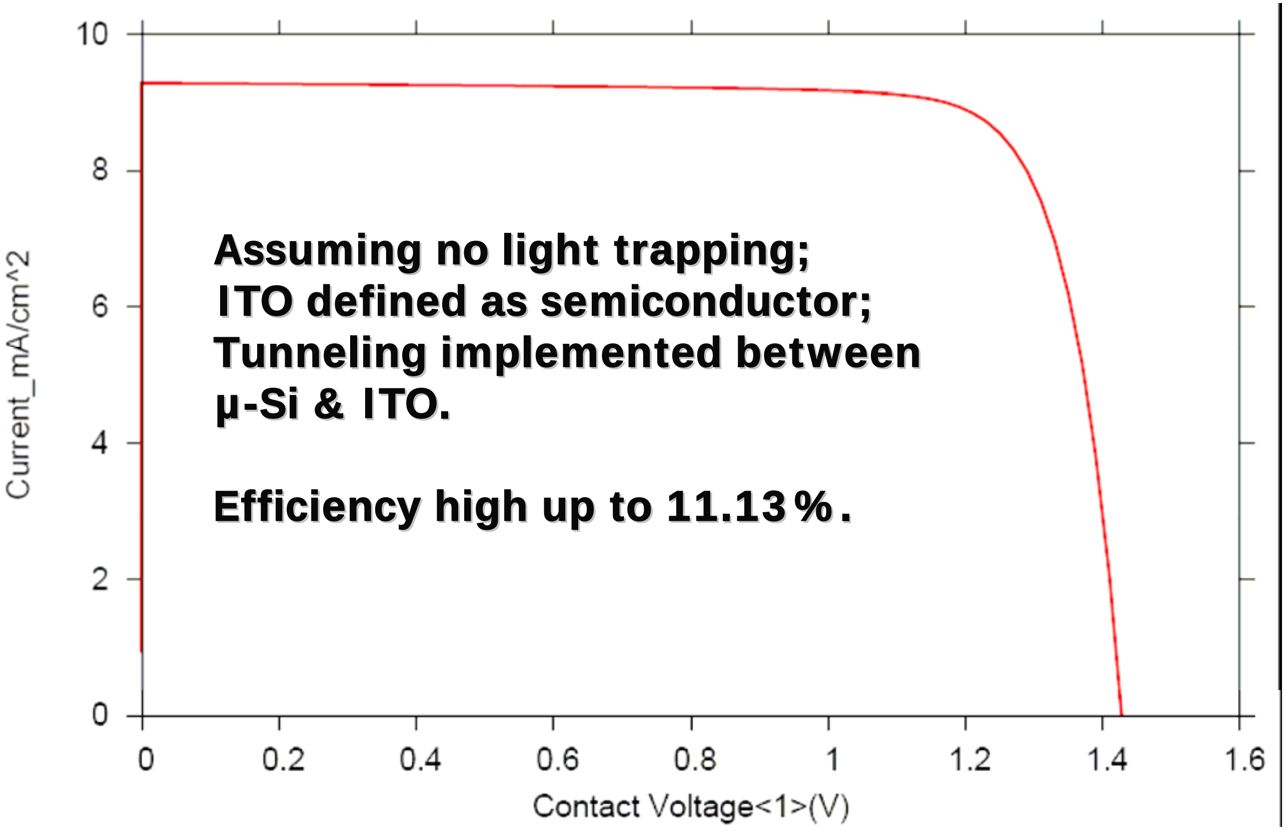
- **At low photon energy region (large wavelength), absorption occurs mainly in the bottom subcell.**
- **At high photon energy region (low wavelength), absorption occurs in both the bottom and top subcells.**

μ-Si/α-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

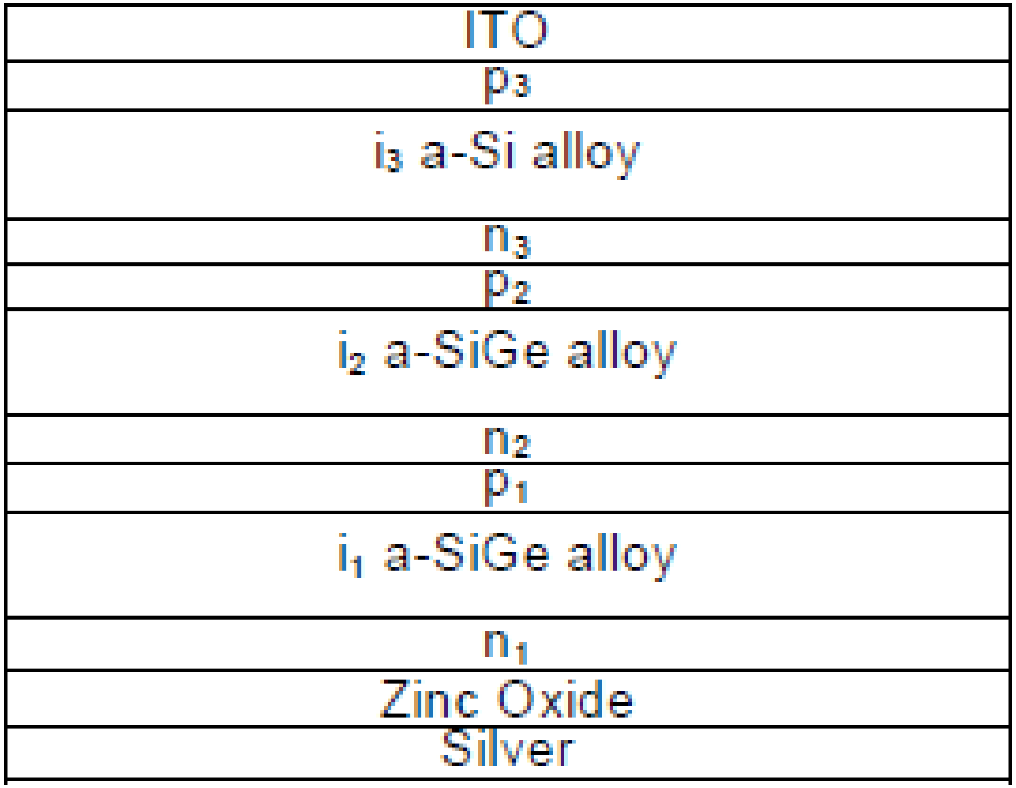


**Assuming no light trapping;
ITO defined as semiconductor;
Tunneling implemented between
μ-Si & ITO.**

Efficiency high up to 11.13%.

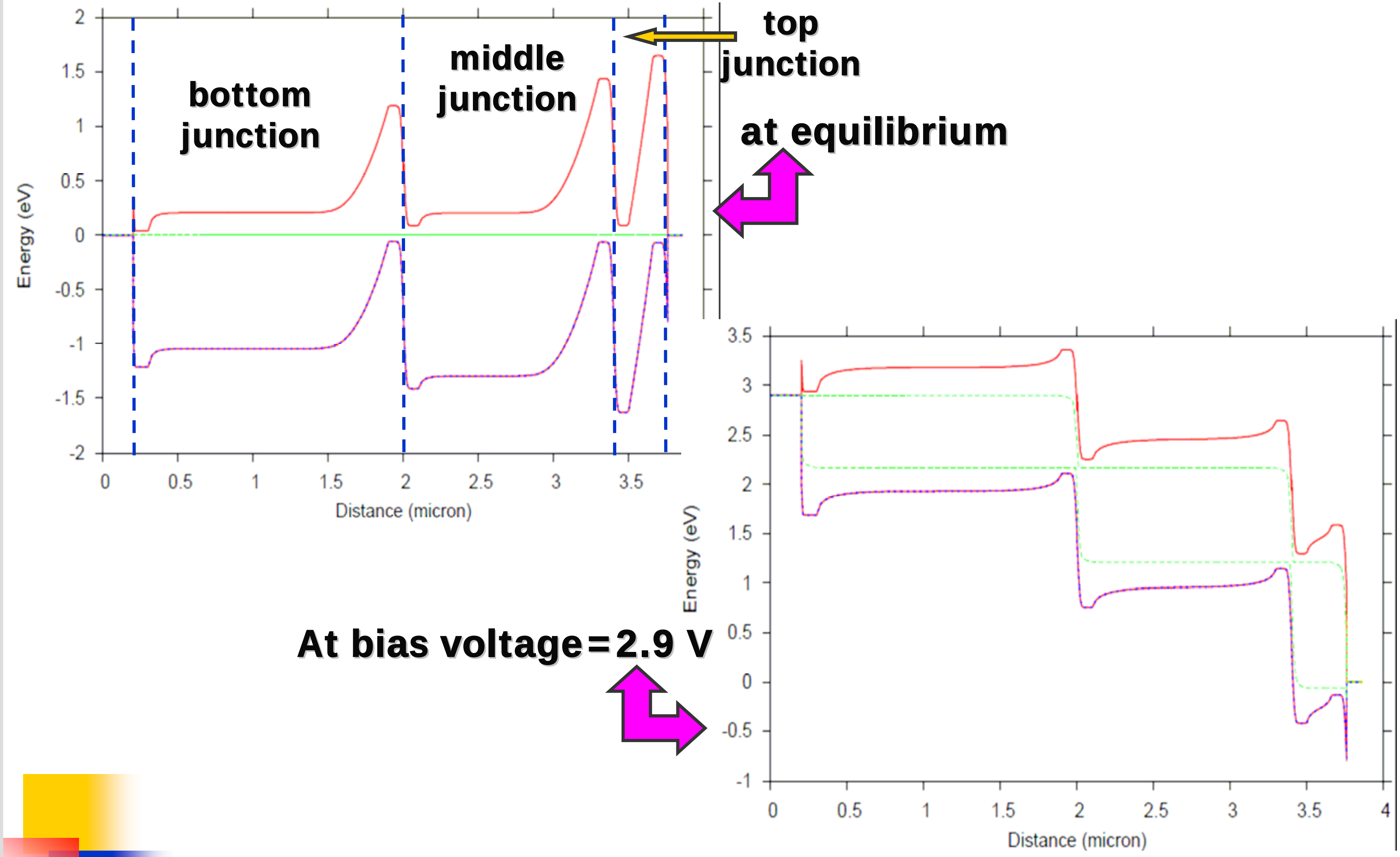
- **Tunneling implemented between top & bottom subcells, also between μ-Si & ITO; Modeling shows higher efficiency.**

α-Si/α-SiGe/α-SiGe TJ tandem cell



- **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: α-Si/α-SiGe/α-SiGe TJ cell



bottom junction

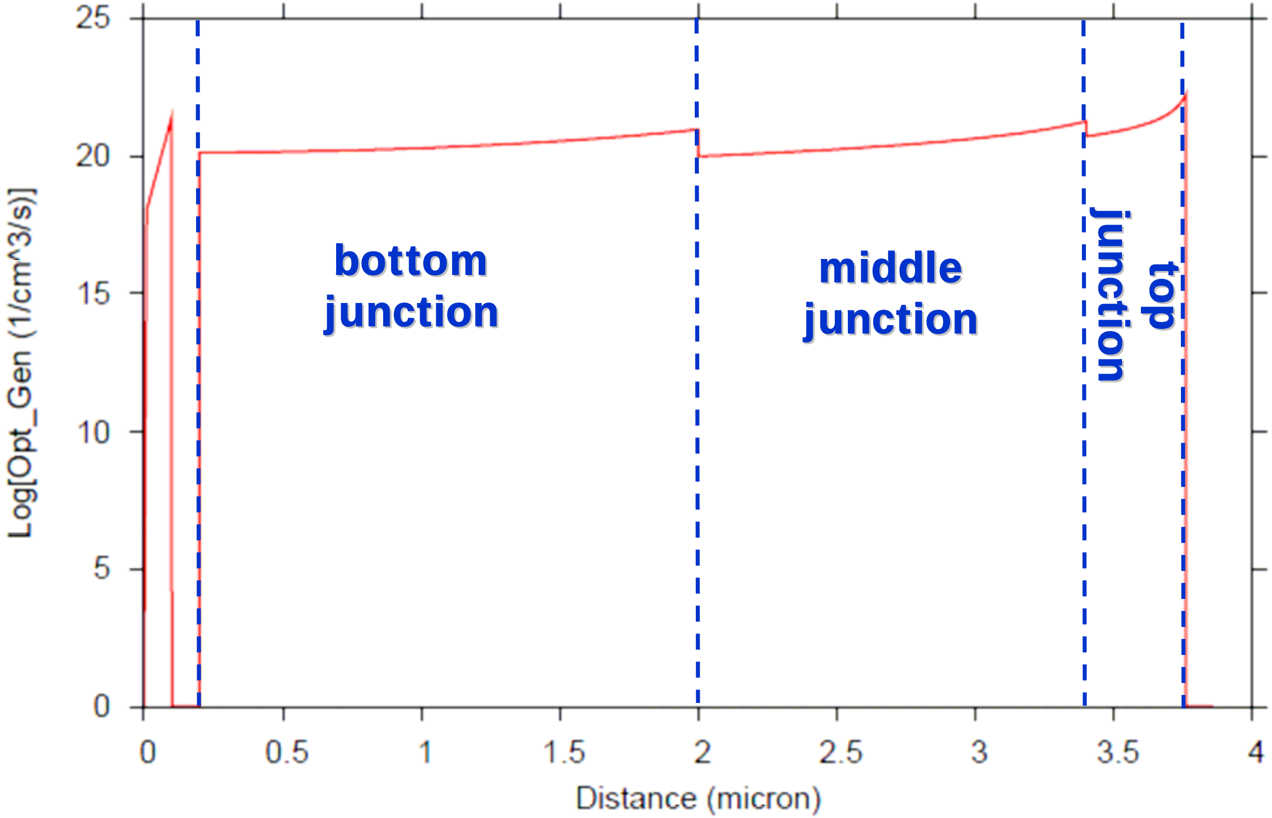
middle junction

top junction

at equilibrium

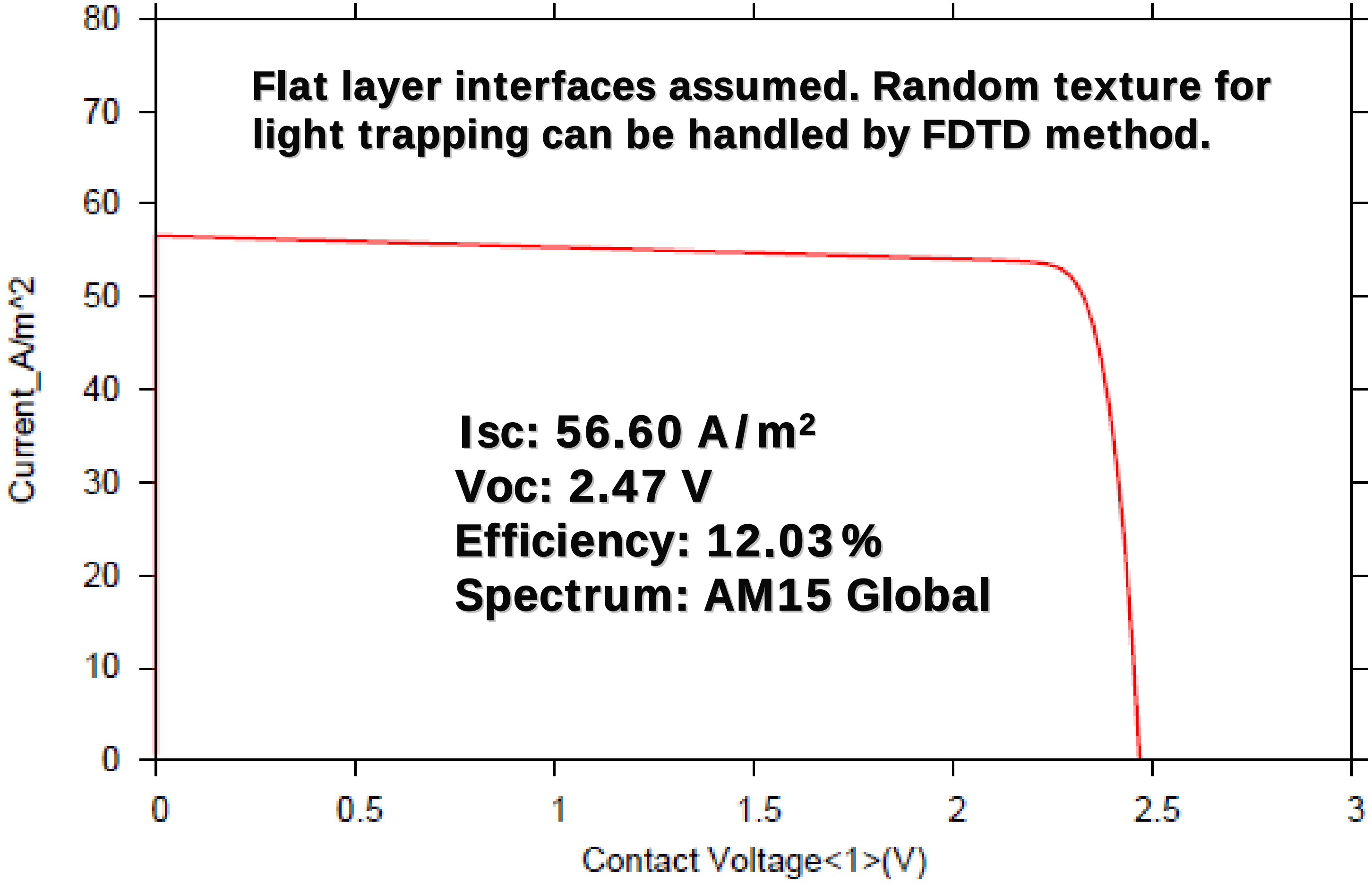
At bias voltage=2.9 V

Optic generation: α-Si/α-SiGe/α-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: α-Si/α-SiGe/α-SiGe TJ cell



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

Isc: 56.60 A/m^2
Voc: 2.47 V
Efficiency: 12.03%
Spectrum: AM15 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.**