

Solar Cells Operation and Modeling

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Outline

- Introduction to Solar Cells
- Absorbing Solar Energy
- Solar Cell Equations Solution
 - PV device characteristics
 - Important generation-recombination mechanisms
 - Analytical model
 - Numerical Solution
 - Shadowing
 - Photon recycling
 - Quantum efficiency for current collection
 - Simulation of Solar Cells with Silvaco

Introduction to Solar Cells

- Historical Developments -

- o 1839: Photovoltaic effect was first recognized by French physicist Alexandre-Edmond Becquerel.
- o 1883: First solar cell was built by Charles Fritts, who coated the semiconductor selenium with an extremely thin layer of gold to form the junctions (1% efficient).
- o 1946: Russell Ohl patented the modern solar cell
- o 1954: Modern age of solar power technology arrives - Bell Laboratories, experimenting with semiconductors, accidentally found that silicon doped with certain impurities was very sensitive to light.
- o The solar cell or photovoltaic cell fulfills two fundamental functions:
 - o Photogeneration of charge carriers (electrons and holes) in a light-absorbing material
 - o Separation of the charge carriers to a conductive contact to transmit electricity

Introduction to Solar Cells

- Solar Cells Types -

- **Homojunction Device**
 - Single material altered so that one side is p-type and the other side is n-type.
 - p-n junction is located so that the maximum amount of light is absorbed near it.
- **Heterojunction Device**
 - Junction is formed by contacting two different semiconductor.
 - Top layer - high bandgap selected for its transparency to light.
 - Bottom layer - low bandgap that readily absorbs light.
- **p-i-n and n-i-p Devices**
 - A three-layer sandwich is created,
 - Contains a middle intrinsic layer between n-type layer and p-type layer.
 - Light generates free electrons and holes in the intrinsic region.

Introduction to Solar Cells

- Solar Cells Generations -

- **First Generation**
 - Single crystal silicon wafers (c-Si)
- **Second Generation**
 - Amorphous silicon (a-Si)
 - Polycrystalline silicon (poly-Si)
 - Cadmium telluride (CdTe)
 - Copper indium gallium diselenide (CIGS) alloy
- **Third Generation**
 - Nanocrystal solar cells
 - Photoelectrochemical (PEC) cells
 - Grätzel cells
 - Polymer solar cells
 - Dye sensitized solar cell (DSSC)
- **Fourth Generation**
 - Hybrid - inorganic crystals within a polymer matrix

Introduction to Solar Cells

- First Generation Solar Cells -

First Generation Photovoltaic cells are the dominant technology in the commercial production of solar cells, accounting for more than 86% of the solar cell market.

- Cells are typically made using a crystalline silicon wafer.
- Consists of a large-area, single layer p-n junction diode.
- Approaches
 - Ingots can be either monocrystalline or multicrystalline.
 - Most common approach is to process discrete cells on wafers sawed from silicon ingots.
 - More recent approach which saves energy is to process discrete cells on silicon wafers cut from multicrystalline ribbons.
- Bandgap $\sim 1.11\text{eV}$

Introduction to Solar Cells

- First Generation Solar Cells -

- **Advantages**

- Broad spectral absorption range.
- High carrier mobilities.

- **Disadvantages**

- Requires expensive manufacturing technologies.
- Growing and sawing of ingots is a highly energy intensive process.
- Fairly easy for an electron generated in another molecule to hit a hole left behind in a previous photo excitation.
- Much of the energy on higher energy photons, at the blue and violet end of the spectrum, is wasted as heat.

Introduction to Solar Cells

- Second Generation Solar Cells -

- **Amorphous silicon cells deposited on stainless-steel ribbon.**
 - Can be deposited over large areas by plasma-enhanced chemical vapor deposition.
 - Can be doped in a fashion similar to c-Si, to form p- or n- type layers.
 - Used to produce large-area photovoltaic solar cells.
 - Bandgap $\sim 1.7\text{eV}$
- **Polycrystalline silicon**
 - Consists solely of crystal silicon grains (1mm), separated by grain boundaries.
 - Main advantage over amorphous Si: mobility of the charge carriers can be magnitudes of order higher.
 - Materials show greater stability under electric field and light-induced stress.
 - Bandgap $\sim 1.1\text{eV}$

Introduction to Solar Cells

- Second Generation Solar Cells -

- **Cadmium Telluride (CdTe) cells deposited on glass.**
 - Crystalline compound formed from cadmium and tellurium with a zinc blende (cubic) crystal structure.
 - Usually sandwiched with cadmium sulfide (CdS) to form a pn junction photovoltaic solar cell.
 - Cheaper than Silicon, especially in thin-film solar technology – not as efficient.
 - Bandgap $\sim 1.58\text{eV}$.
- **Copper gallium indium diselenide (CIGS) solar cells**
 - Deposited on either glass or stainless steel substrates.
 - More complex heterojunction model.
 - Bandgap $\sim 1.38\text{eV}$.

Introduction to Solar Cells

- Second Generation Solar Cells -

- **Advantages**

- Lower manufacturing costs.
- Lower cost per watt can be achieved.
- Reduced mass.
- Less support is needed when placing panels on rooftops.
- Allow fitting panels on light or flexible materials, even textiles.

- **Disadvantages**

- Typically, the efficiency of thin-film solar cells are lower compared with silicon (wafer-based) solar cells.
- Amorphous silicon is not stable.
- Increased toxicity.

Introduction to Solar Cells

- Third Generation Solar Cells -

- Very different from the previous semiconductor devices.
- Do not rely on a traditional pn- junction to separate photo generated charge carriers.
- Devices include
 - Nanocrystal Solar Cells.
 - Photo electrochemical cells
 - Graetzel cell
 - Dye-sensitized hybrid solar cells.
 - Polymer solar cells.

Introduction to Solar Cells

- Third Generation Solar Cells -

- **Advantages**

- Low Energy, High throughput processing technologies.
- Polymer cells- solution processable, chemically synthesized.
- Polymer cells- Low material cost
- Graetzel cells- attractive replacement for existing technologies in “low density” applications like rooftop solar collectors.
- Graetzel cells- Works even in low-light conditions.
- DSSC- Potentially rechargeable.

- **Disadvantages**

- Efficiency is lower compared to silicon (wafer-based) solar cells.
- Polymer solar cells
 - Degradation effects: efficiency is decreased over time due to environmental effects.
 - High Bandgap.
- PEC cells undergo degradation of the electrodes from electrolyte.

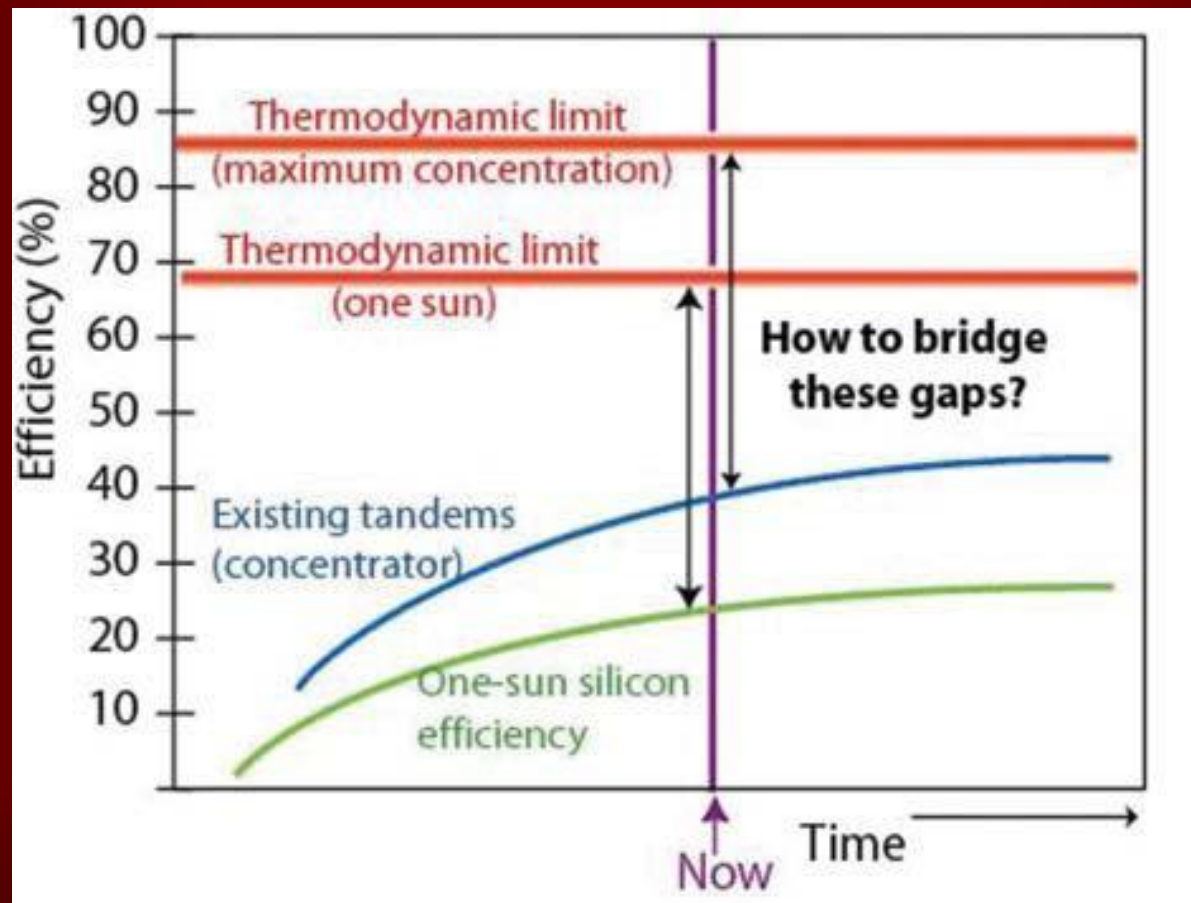
Introduction to Solar Cells

- Fourth Generation Solar Cells -

- Thin multi-spectrum layers can be stacked to make multi-spectrum solar cells
 - Layer that converts different types of light is first.
 - Another layer for the light that passes.
 - Lastly is an infra-red spectrum layer for the cell.
 - Converting some of the heat for an overall solar cell composite.
 - More efficient and cheaper.
 - Based on polymer solar cell and multi junction technology.
- Future advances will rely on new nanocrystals, such as cadmium telluride tetrapods.
 - Potential to enhance light absorption and further improve charge transport.
- Gains can be made by incorporating application-specific organic components, including electro active surfactants which control the physical & electronic interactions between polymer and nanocrystals.

Introduction to Solar Cells

- **Narrowing gap between Existing and Theoretical PV efficiencies -**



Introduction to Solar Cells

- Technological Improvements -

- **Multijunction Devices**

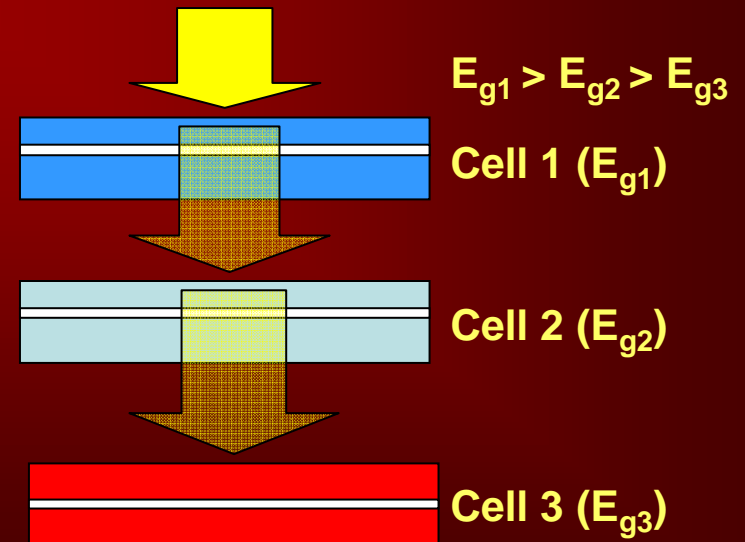
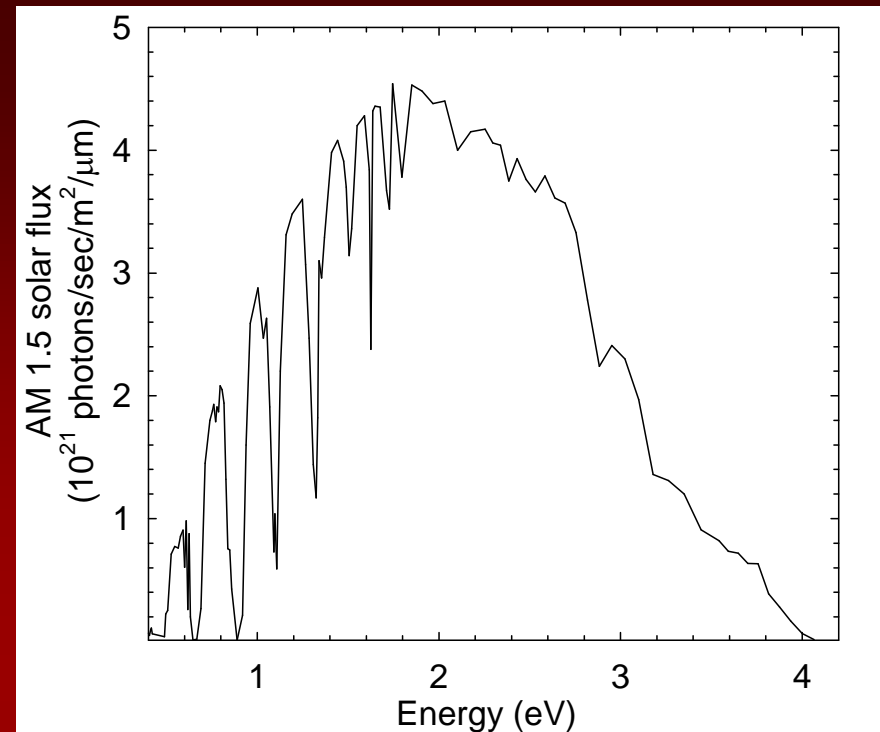
- Stack of individual single junction cells in descending order of bandgap.
- Top cell captures high energy photons and passes rest on to lower bandgap cells.
- Mechanical stack:
 - Two individual solar cells are made independently.
 - Then are mechanically stacked, one on top of another.
- Monolithic stack:
 - One complete solar cell is made first.
 - Layers of subsequent cells are grown or deposited.
- Example: GaAs Multijunction
 - Triple junction cells of semiconductors: GaAs, Ge and GaInP₂.

- Intrinsic efficiency limit for a solar cell using a single semiconducting material is 31%.

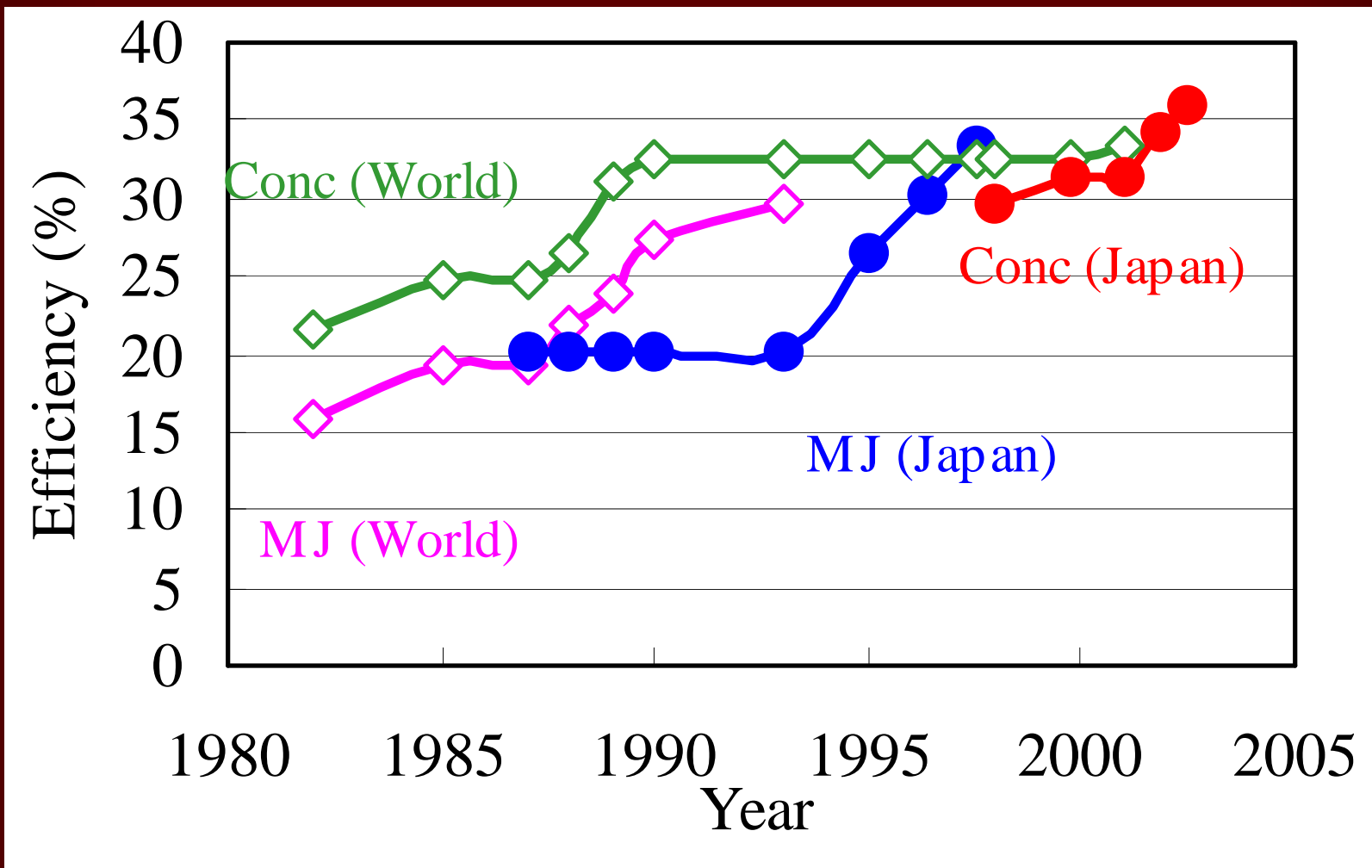
- Light with energy below the bandgap of the semiconductor will not be absorbed
- The excess photon energy above the bandgap is lost in the form of heat.
- Single crystal GaAs cell: 25.1% AM1.5, 1x

- Multijunction (MJ) tandem cell

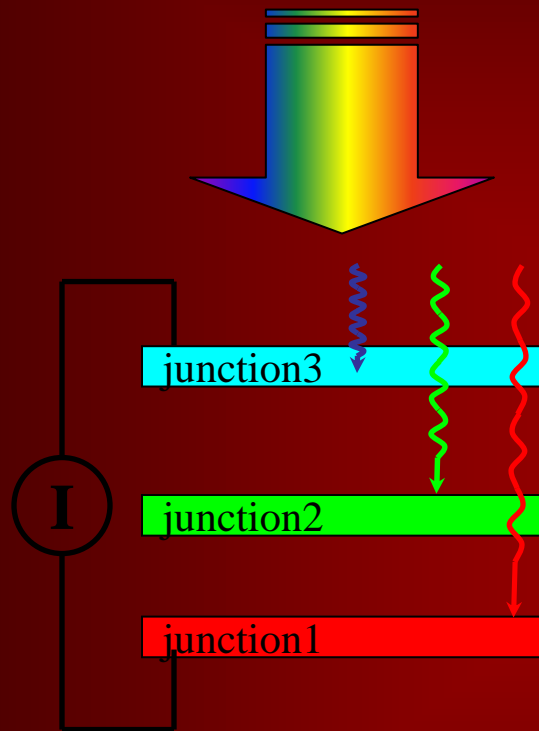
- Maximum thermodynamically achievable efficiencies are increased to 50%, 56%, and 72% for stacks of 2, 3, and 36 junctions with appropriately optimized energy gaps



State-of-the art 3-junction GaInP/Ga(In)As/Ge solar cell: 36 % efficient

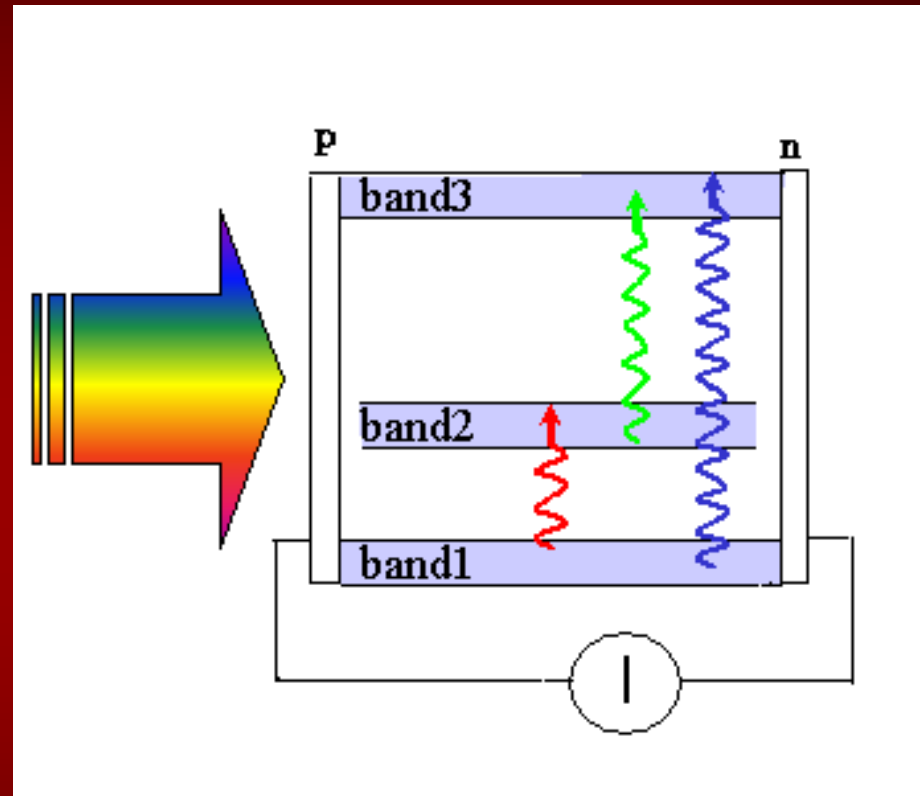


Multijunction vs. Multiband



Multi-junction

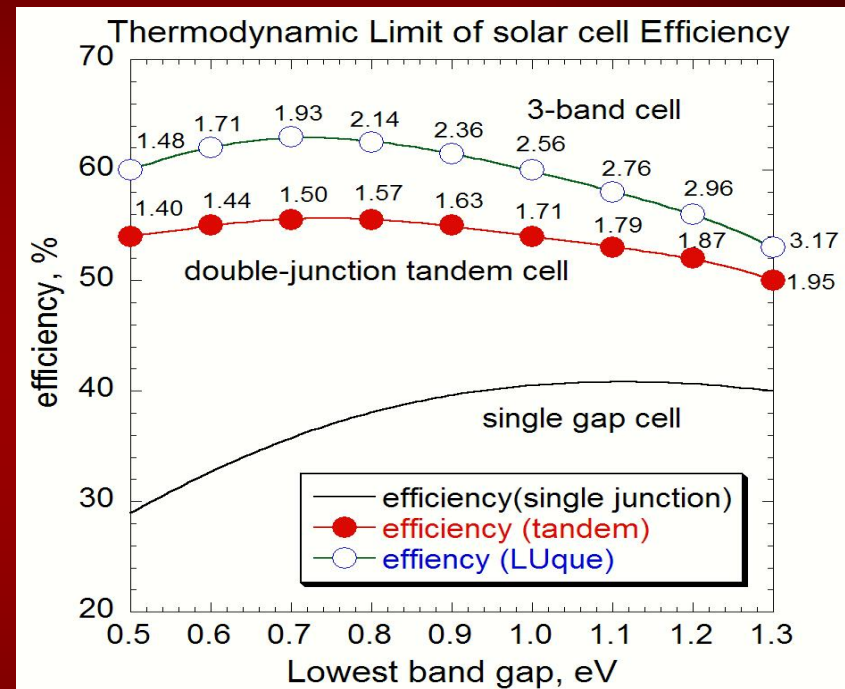
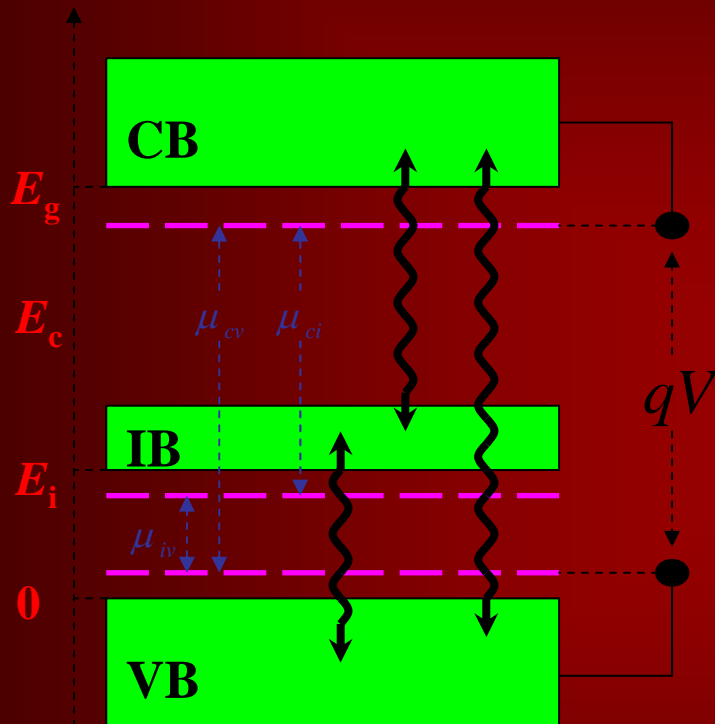
- Single gap (two bands) each junction
- N junctions \Rightarrow N absorptions
- Efficiency ~30-40%



Multi-band

- Single junction (no lattice-mismatch)
- N bands \Rightarrow $N \cdot (N-1)/2$ gaps
 \Rightarrow $N \cdot (N-1)/2$ absorptions
- Add one band \Rightarrow add N absorptions

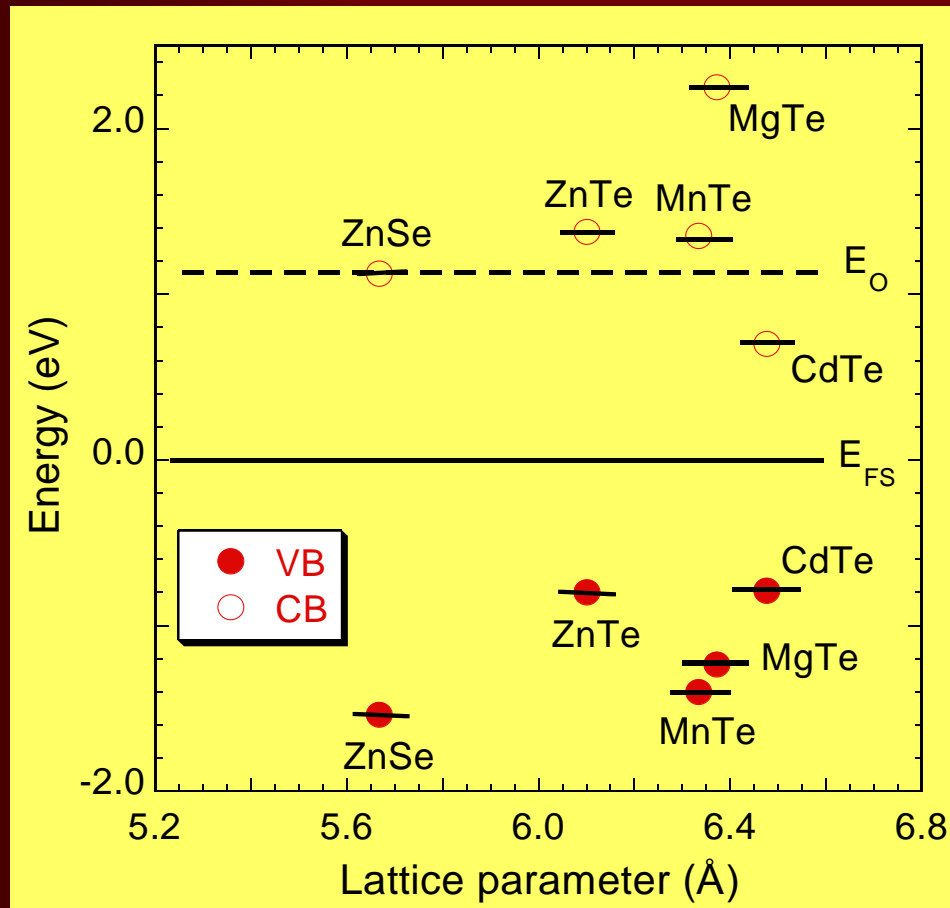
Theoretical efficiency of Intermediate band solar cells



- Intermediate Band Solar Cells can be very efficient
 - Max. efficiency for a 3-band cell=63%
 - Max. efficiency for a 4-band cell=72%
 - In theory, better performance than any other ideal structure of similar complexity

But NO multi-band materials realized to date

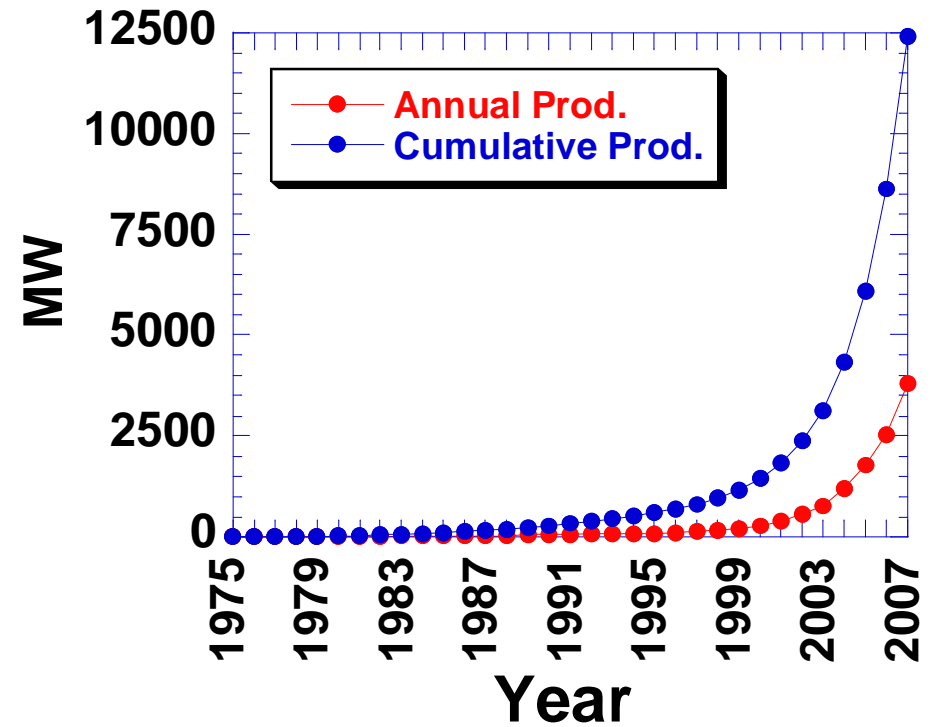
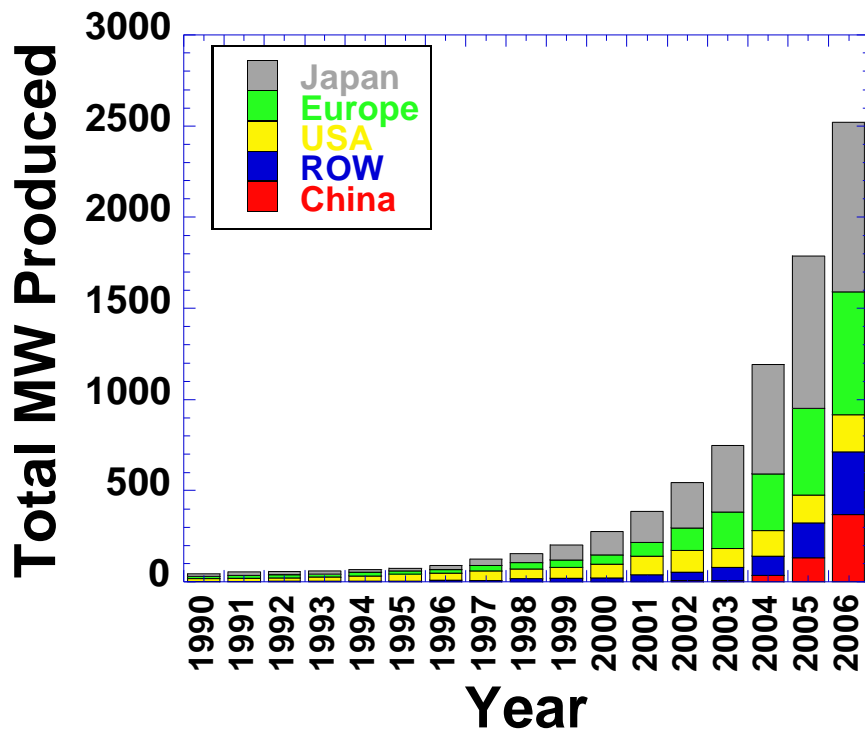
Highly Mismatched Alloys for Multiband Cells



- Oxygen in II-VI compounds has the requisite electronegativity and atomic radius difference
 - $X_{\text{O}} = 3.44$; $R_{\text{O}} = 0.073 \text{ nm}$
 - $X_{\text{S}} = 2.58$; $R_{\text{S}} = 0.11 \text{ nm}$
 - $X_{\text{Se}} = 2.55$; $R_{\text{Se}} = 0.12 \text{ nm}$
 - $X_{\text{Te}} = 2.1$; $R_{\text{Te}} = 0.14$
- Oxygen level in ZnTe is 0.24 eV below the CB edge
 - *Can this be used to form an intermediate band?*
- **Synthesis**
 - Very low solid solubility limits of O in II-VI compounds
 - Nonequilibrium synthesis required

Introduction to Solar Cells

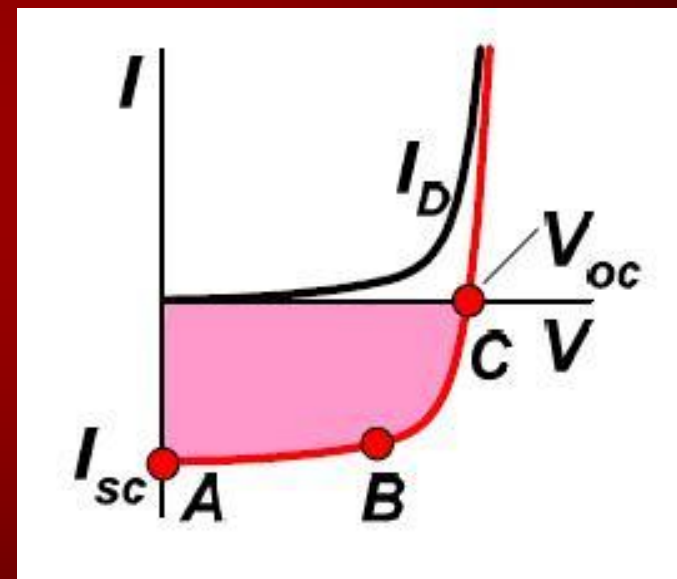
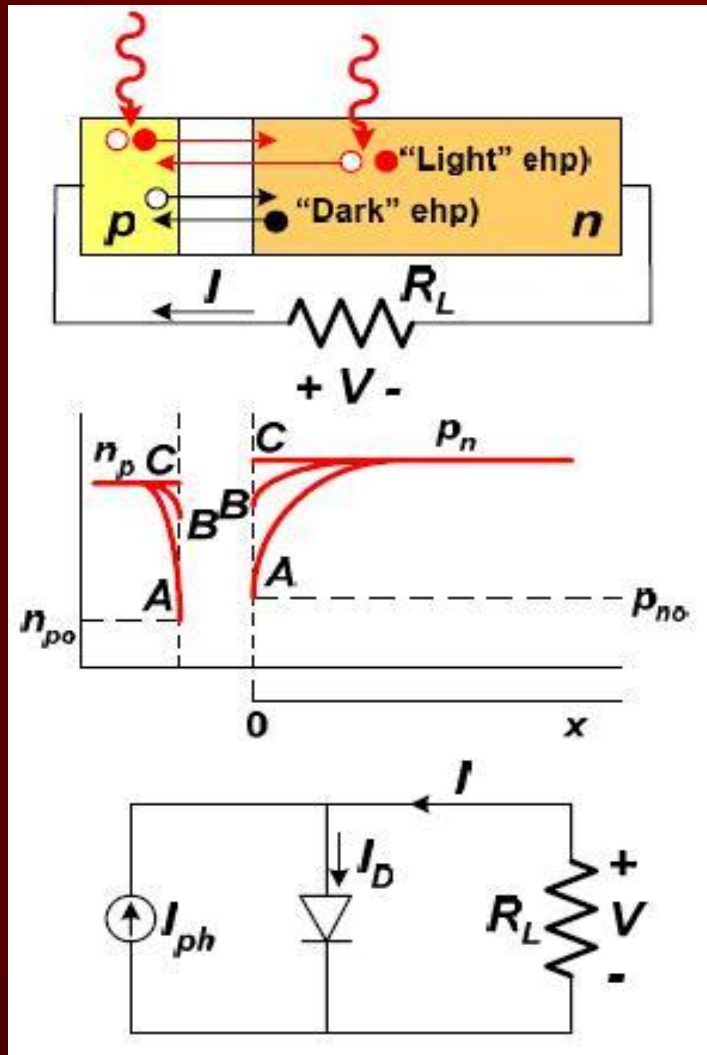
- PV Costs and Shipments -



Compiled by Earth Policy Institute from Worldwatch Institute

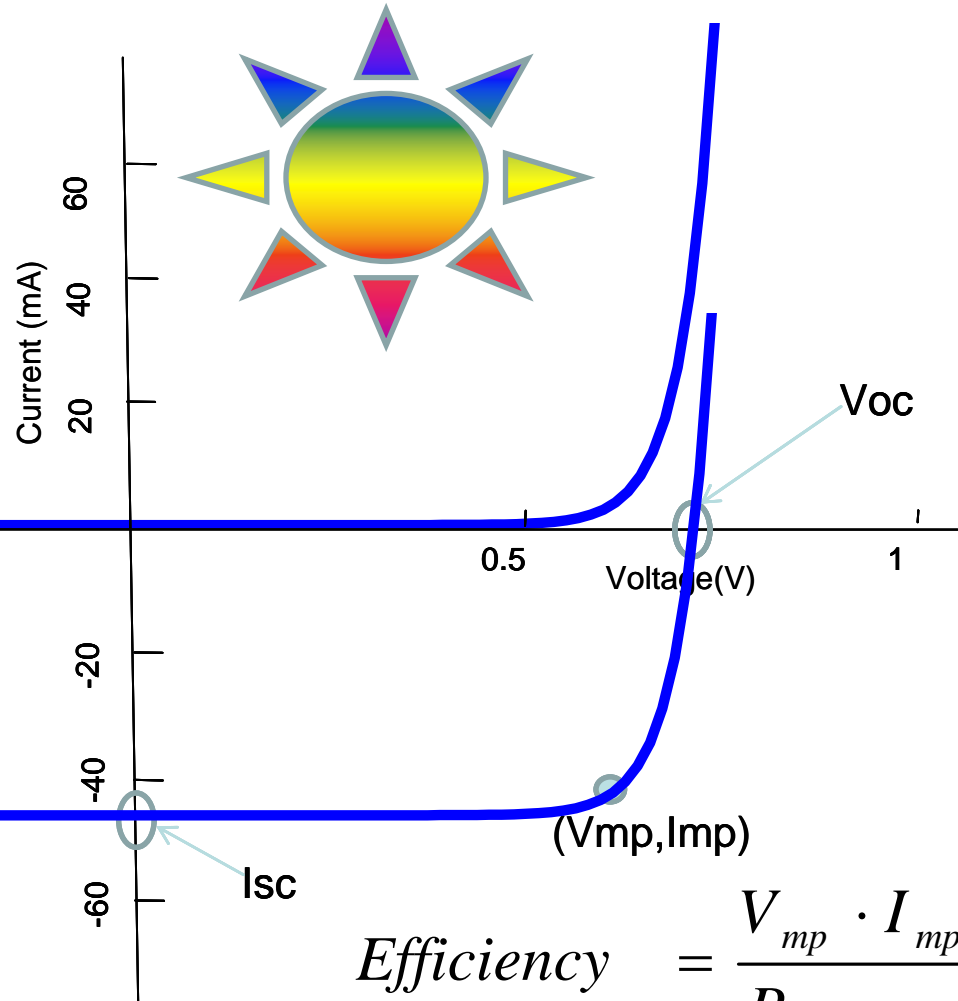
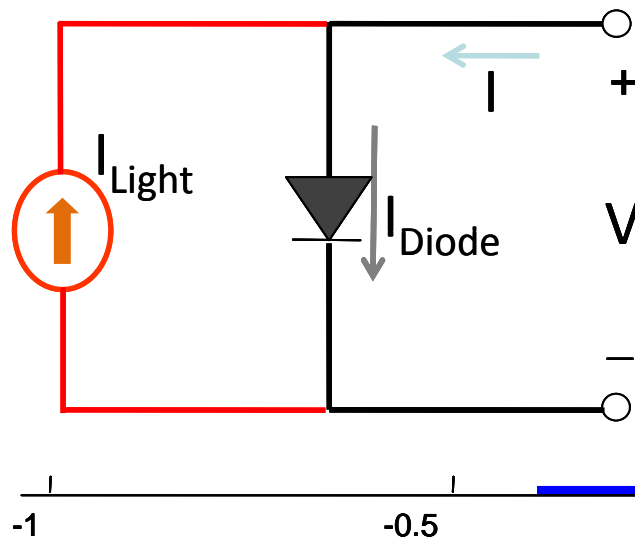
Introduction to Solar Cells

- Principle of Operation -



Introduction to Solar Cells

- IV Curve of a Well Behaved Solar Cell -



$$I_{Diode} = I_0 \cdot \left(\exp \frac{q \cdot V}{kT} - 1 \right)$$

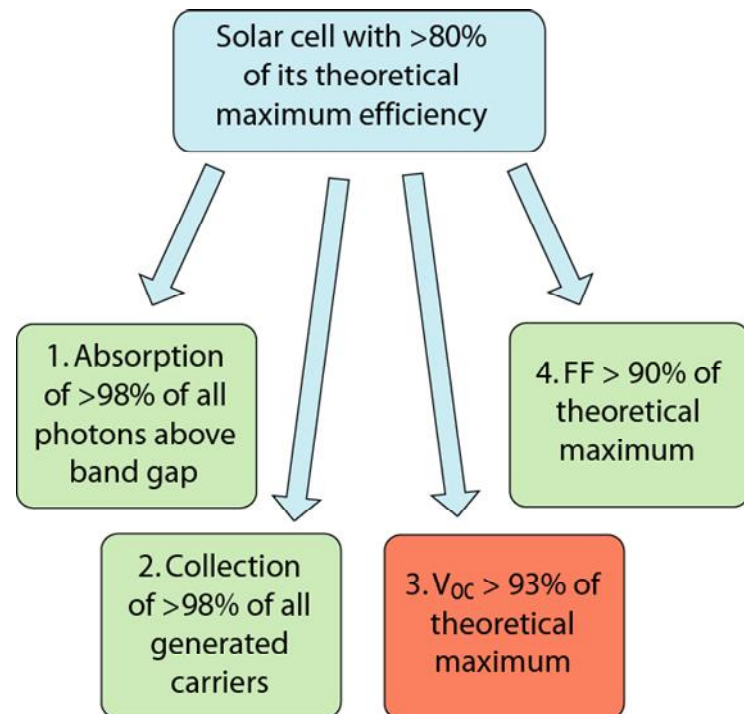
$$I = I_0 \cdot \left(\exp \frac{q \cdot V}{kT} - 1 \right) - I_{Light}$$

$$Efficiency = \frac{V_{mp} \cdot I_{mp}}{Power_{in}}$$

Introduction to Solar Cells

- Design Rules for High Performance -

- For a high solar cell efficiency, simultaneously need high absorption, collection, open circuit voltage and fill factor.
- Absorption and collection are typically achievable by “clever” engineering & innovation.
- Voltage is controlled by worst, localized region, NOT the same region which absorbs the light – this is fundamentally why single crystal solar cells are highest efficiency.**
- Predictive models and design rules for all characteristics are necessary for the device parameters.



Introduction to Solar Cells

- Maximizing Efficiency -

$$\eta = \frac{I_{sc} V_{oc} FF}{P_{in}}$$

↑ I_{sc}

- ↓ E_G
- ↓ Reflection
 - Surface
 - Metal
- ↑ L_n, L_p
- ↓ S_r
- x_j optimum

↑ V_{oc}

- ↑ E_G
- ↑ doping
- ↑ L_n, L_p
- ↓ S_r

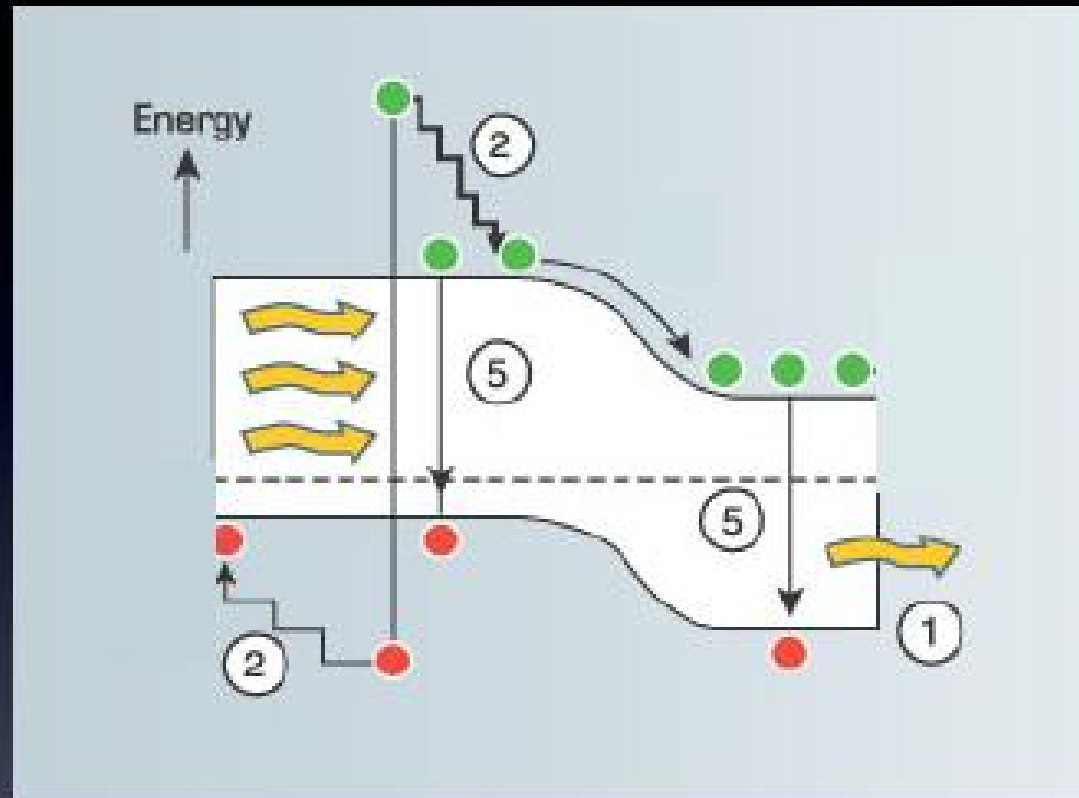
Doping and diffusion length are related

↑ FF

- ↓ Series R
 - Metal
 - Emitter
 - ↑ doping
 - Thick emitter

Introduction to Solar Cells

- Solar Cell Losses -



Intrinsic losses:

(1 and 2) - due to mismatch of E_g and photon energy

(5) - radiative recombination

Introduction to Solar Cells

- Solar Cell Panels -

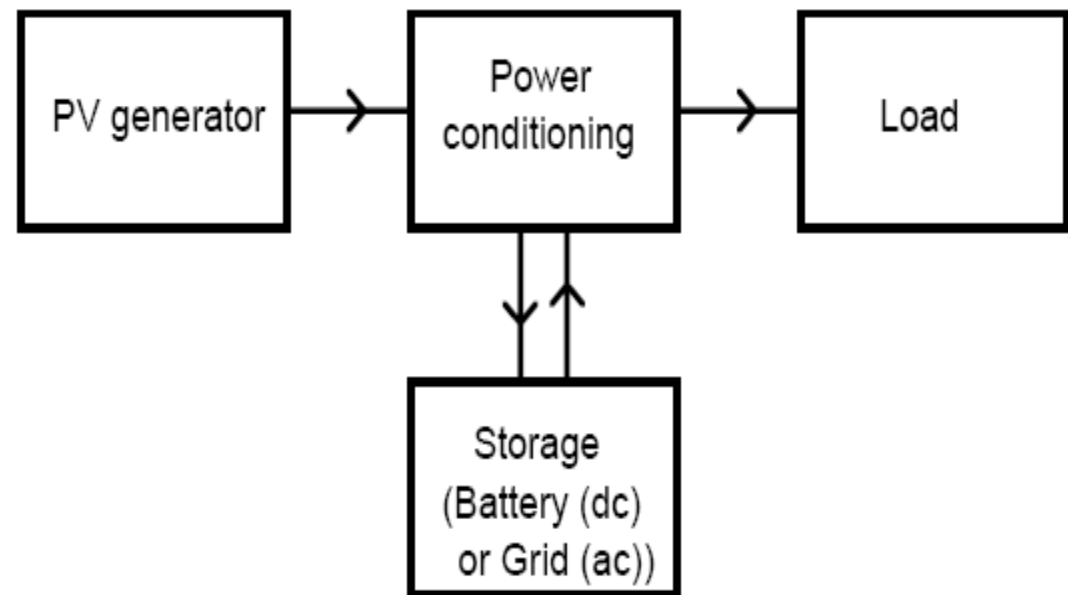
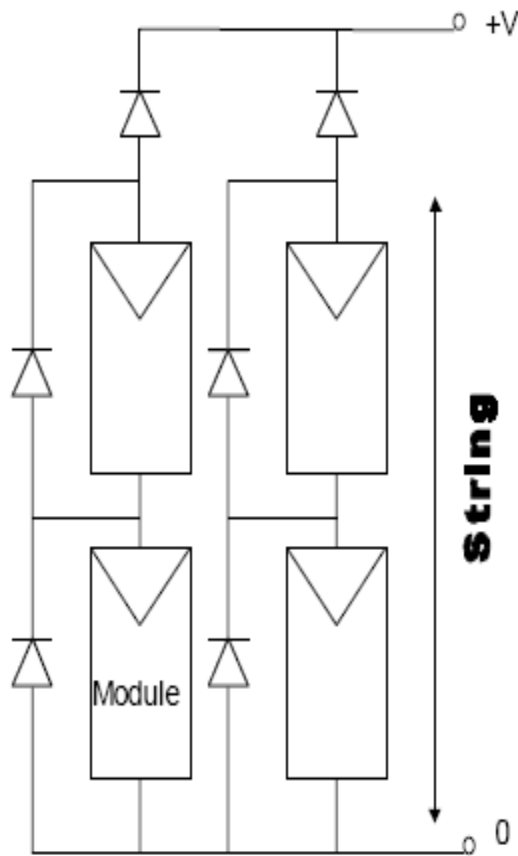


HOME DEPOT

Sunforce 130 Watt Solar Panel Kit
Model # 39307 Internet/Catalog # 100677617
\$9,999.97/EA-Each

Introduction to Solar Cells

- Solar Cell Panels -



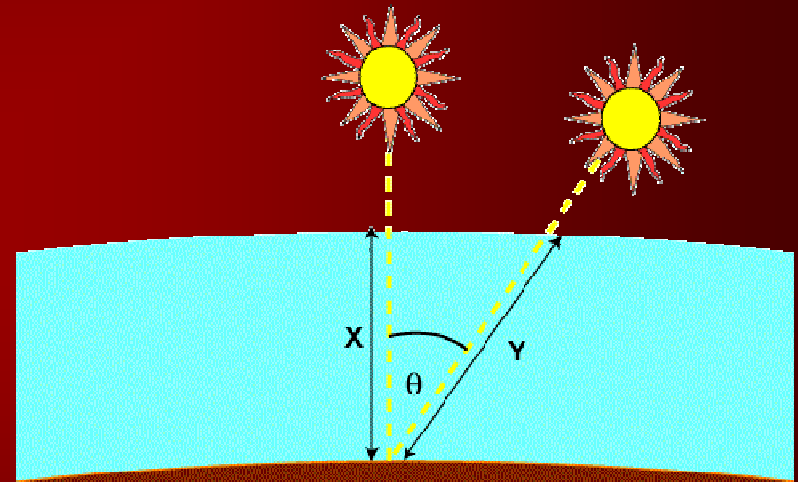
Absorbing Solar Energy

- Air Mass -

The Air Mass is the path length which light takes through the atmosphere normalized to the shortest possible path length (that is, when the sun is directly overhead). The Air Mass quantifies the reduction in the power of light as it passes through the atmosphere and is absorbed by air and dust. The Air Mass is defined as:

$$AM = \frac{1}{\cos(\theta)}$$

where θ is the angle from the vertical (zenith angle). When the sun is directly overhead, the Air Mass is 1.



Absorbing Solar Energy

- Air Mass 1.5 -

Solar panels do not generally operate under one atmosphere's thickness, if the sun is at an angle to the Earth's surface the effective thickness will be greater.

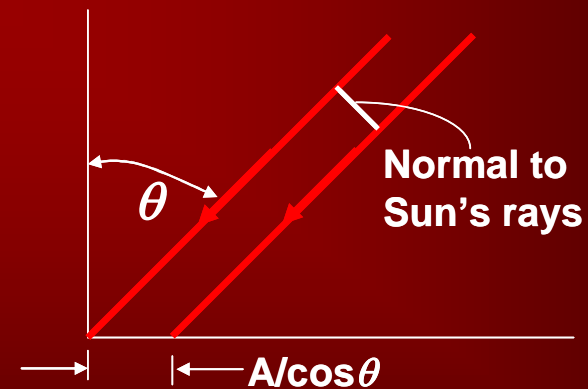
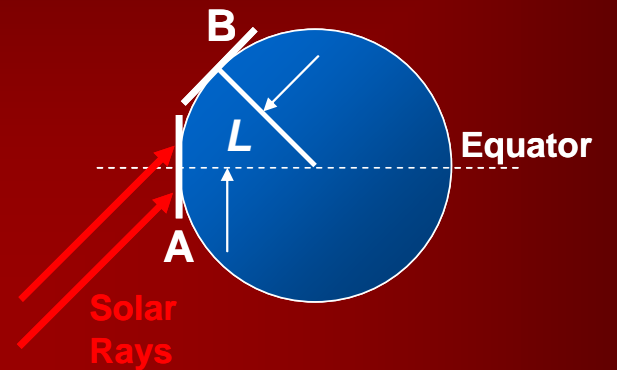
Since solar cell development is concentrated in the United States, Europe and Japan, an AM number representing the spectrum at mid-latitudes is much more common.

"AM1.5", 1.5 atmosphere thicknesses, corresponds to a solar zenith angle of 48.2° , and is almost universally used to characterize terrestrial solar panels.

Absorbing Solar Energy

- Tilt Angle -

- Planes A and B:
 - ◆ Horizontal on earth surface
- For B to be parallel to A, must be tilted by angle L (latitude angle)
- Northern hemisphere
 - ◆ Panel should face south at angle $L+10^\circ$
- Phoenix: $L = 33.5^\circ$

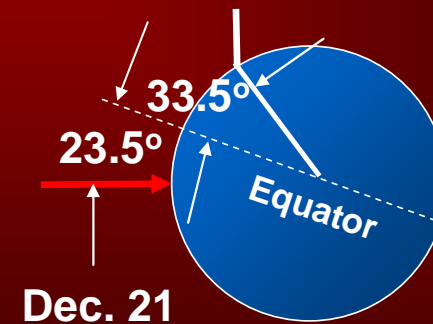
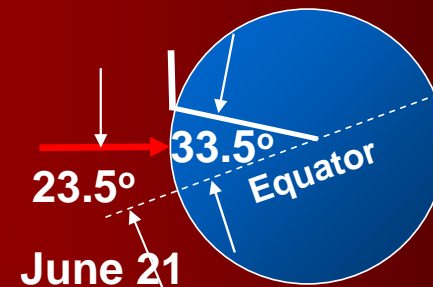
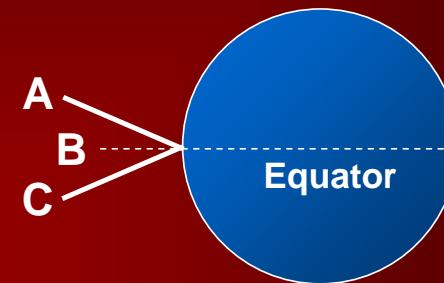


Intensity on earth = $A \cos \theta$

Absorbing Solar Energy

- Angle of Declination -

- The solar array can be made perpendicular to the sun every day
- Sun path length through atmosphere increases
- $D_s = 1$ (Dec. 21); $= 365$ (Dec. 20)
- A: Dec. 21; $\delta = -23.45^\circ$
- B: March/Sept. 21; $\delta = 0$
- C: June 21; $\delta = 23.45^\circ$
- June 21: tilt = $10^\circ = 33.5^\circ - 23.5^\circ$
- Dec. 21: tilt = $57^\circ = 33.5^\circ + 23.5^\circ$



Absorbing Solar Energy

- USA Power Consumption -

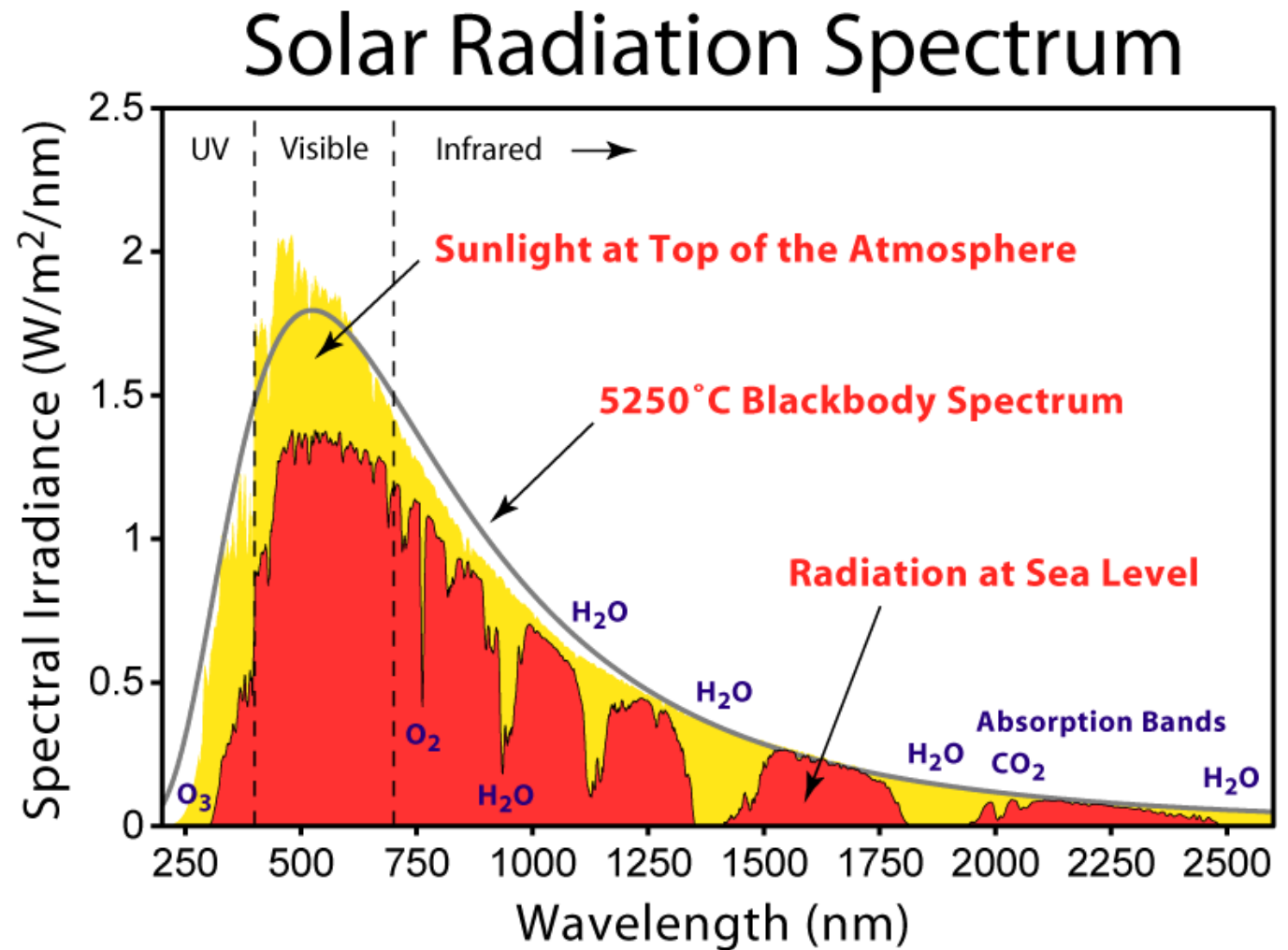
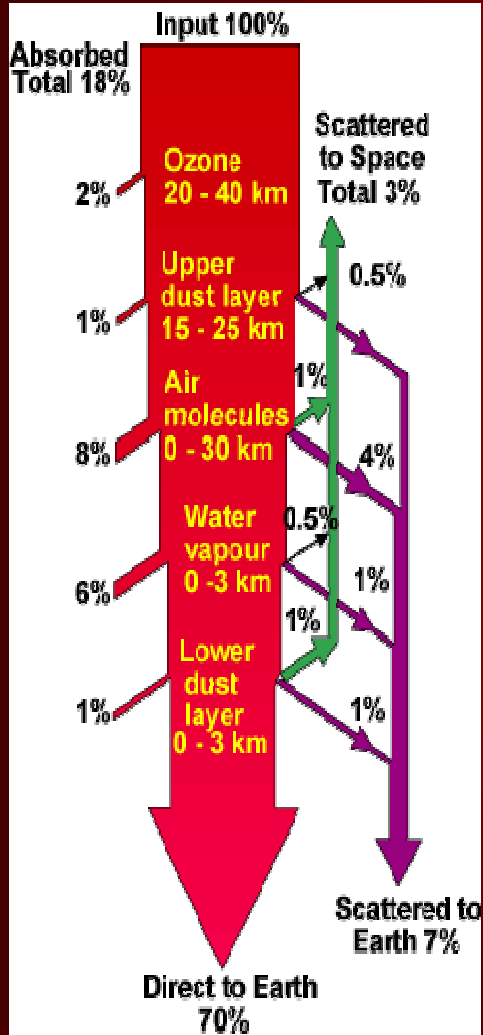
What area is required to supply all of the US electrical power by solar cells?

- US power consumption in 2005:
 $\sim 4 \times 10^{15}$ W-h
- Sun power ≈ 1000 W/m²
- Solar cell $\eta = 15\% \Rightarrow 150$ W/m²
- Sun shines ~ 7 hours/day
 $\Rightarrow 150 \times 3650$ W-h/m²
- Need 3.8×10^5 W-h/m² $\times A$
 $= 4 \times 10^{15}$ W-h $\Rightarrow A \approx 10^{10}$ m²
- For square area $A = d^2 = 10^{10}$ m²
- $\Rightarrow d = 100$ km or $d \approx 60$ miles
- With space between solar panels
 $\Rightarrow d \approx 100$ miles
- 2007 IC Si: 1.5×1.5 miles²



Absorbing Solar Energy

- Solar Spectrum -



Absorbing Solar Energy

- Solar Spectrum -

- The spectrum outside the atmosphere, the 5,800 K black body, is referred to as "AM0", meaning "zero atmospheres". Cells used for space power applications, like those on [communications satellites](#) are generally characterized using AM0.
- The spectrum after traveling through the atmosphere to [sea level](#) with the sun directly overhead is referred to as "AM1". This means "one atmosphere". Conveniently, silicon solar cells are not very sensitive to the portions of the spectrum lost in the atmosphere. The resulting spectrum more closely matches the [bandgap](#) of [silicon](#) so silicon solar cells are more efficient at AM1 than AM0.
- Solar panels do not generally operate under one atmosphere's thickness, if the sun is at an angle to the Earth's surface the effective thickness will be greater. Since solar cell development is concentrated in the United States, Europe and Japan, an AM number representing the spectrum at mid-latitudes is much more common. "AM1.5", 1.5 atmosphere thicknesses, corresponds to a solar zenith angle of 48.2° , and is almost universally used to characterize terrestrial solar panels.

Absorbing Solar Energy

- Optical Properties of Solar Cell Materials -

- **Absorption Coefficient**

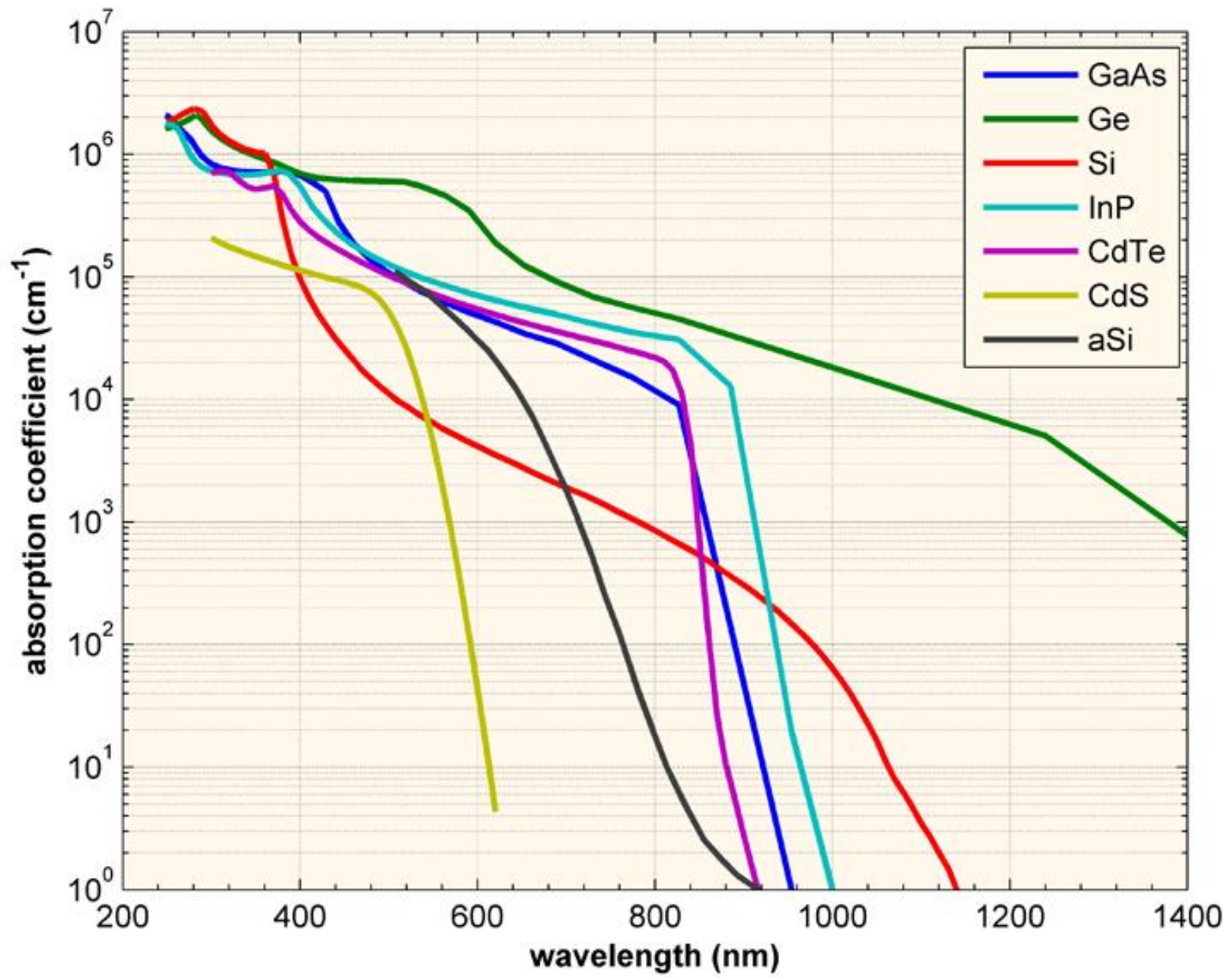
- The absorption coefficient determines how far into a material light of a particular wavelength can penetrate before it is absorbed.

- In a material with a low absorption coefficient, light is only poorly absorbed, and if the material is thin enough, it will appear transparent to that wavelength.

- The absorption coefficient depends on the material and also on the wavelength of light which is being absorbed.

- Semiconductor materials have a sharp edge in their absorption coefficient, since light which has energy below the band gap does not have sufficient energy to raise an electron across the band gap.

Consequently this light is not absorbed.



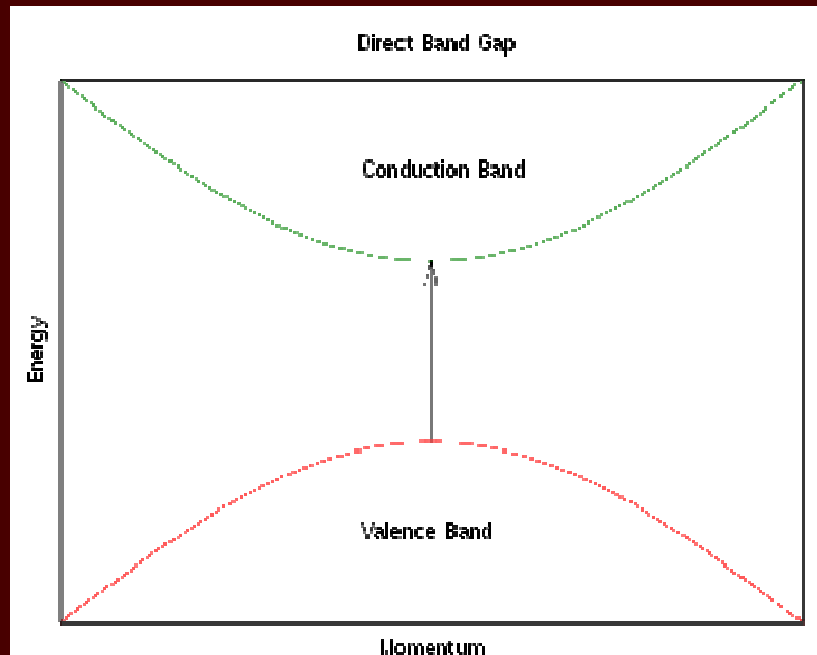
Absorption coefficient is defined as:

$$\alpha = \frac{4\pi k}{\lambda}$$

where λ is the wavelength. If λ is in nm, multiply by 10^7 to get the absorption coefficient in the units of cm^{-1} .

The measured intensity I of transmitted through a layer of material with thickness x is related to the incident intensity I_0 according to the inverse exponential power law that is usually referred to as [Beer–Lambert law](#):

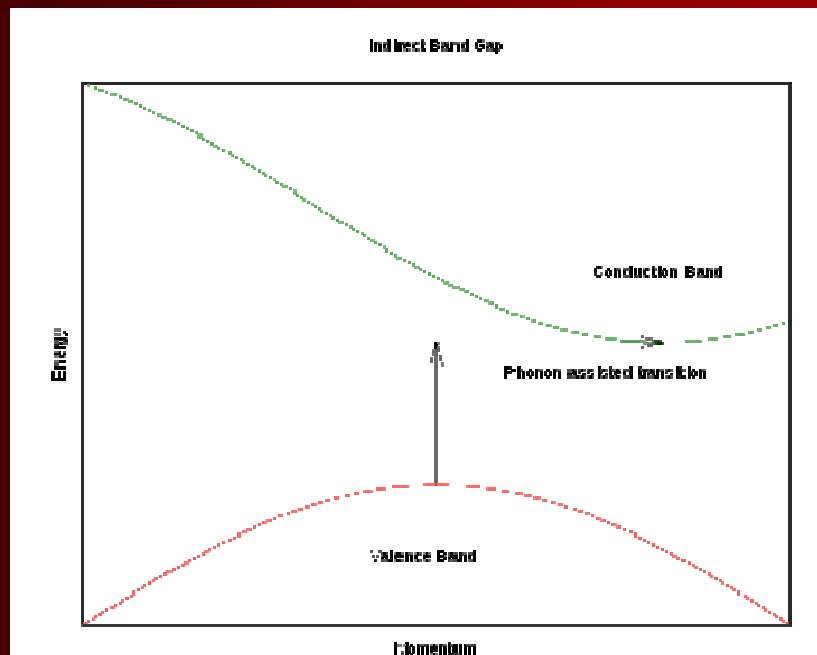
$$I = I_0 e^{-\alpha x}$$



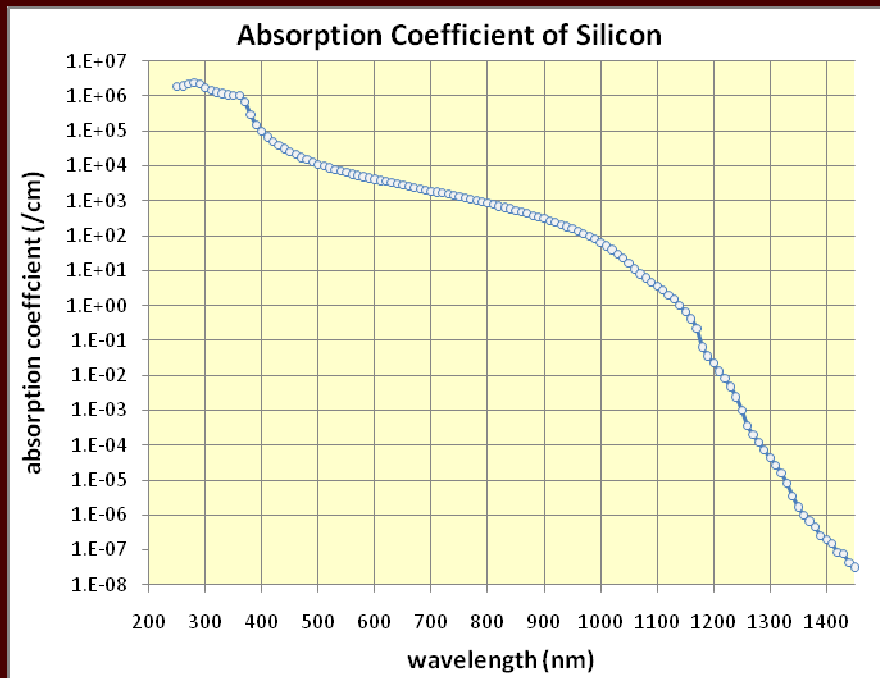
$$\alpha \approx A^* \sqrt{h\nu - E_g}$$

$$A^* = \frac{q^2 x_{vc}^2 (2m_r)^{3/2}}{\lambda_0 \epsilon_0 \hbar^3 n}$$

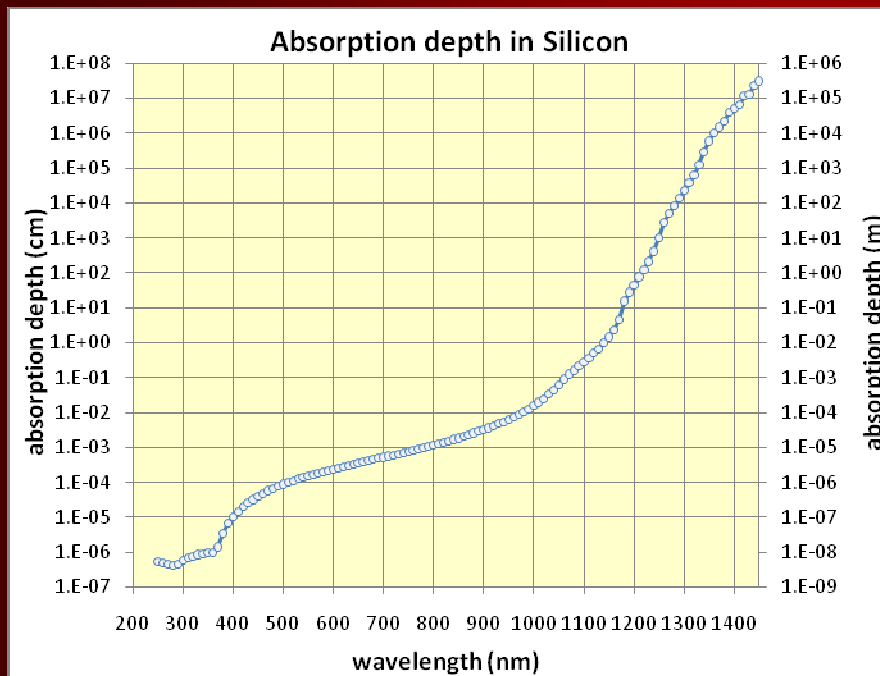
$$m_r = \frac{m_h^* m_e^*}{m_h^* + m_e^*}$$



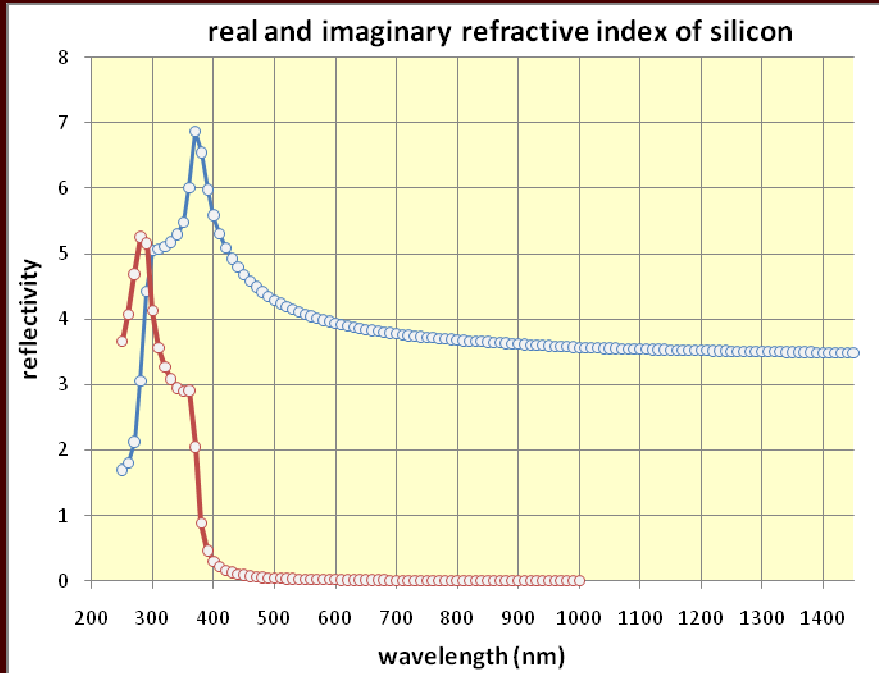
$$\alpha \propto \frac{(h\nu - E_g + E_p)^2}{\exp(\frac{E_p}{kT}) - 1} + \frac{(h\nu - E_g - E_p)^2}{1 - \exp(-\frac{E_p}{kT})}$$



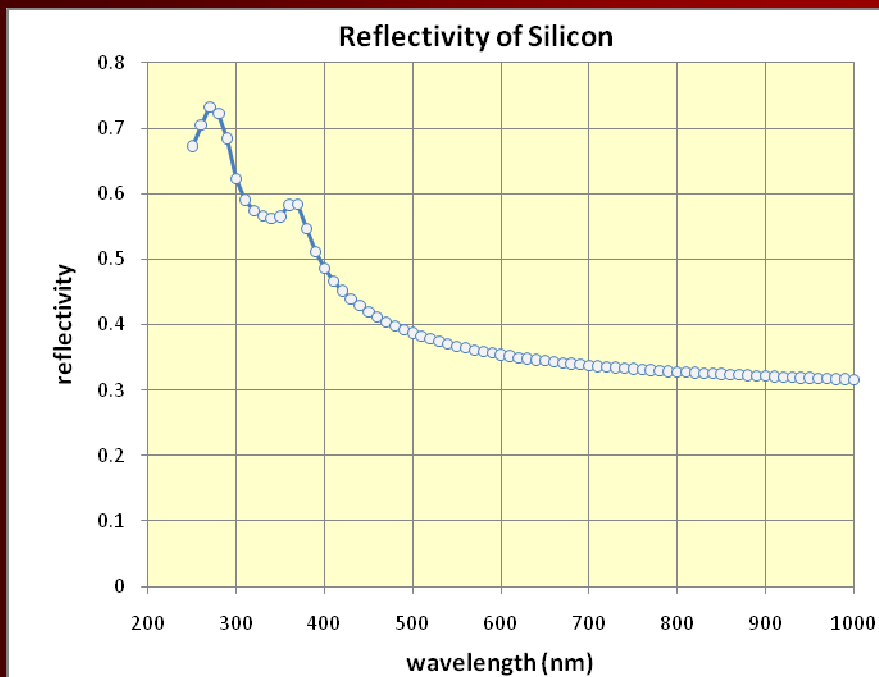
Absorption coefficient of silicon in cm⁻¹ as a function of the wavelength. Silicon is an indirect bandgap semiconductor so there is a long tail in absorption out to long wavelengths. The data is graphed on a log scale. The drop in absorption at the band gap (around 1100 nm) is sharper than might first appear.



The absorption depth is the inverse of the absorption coefficient. An absorption depth of, for example, 1 μ m means that the light intensity has fallen to 36% (1/e) of its original value.



Real and (negative) imaginary components of the refractive index for silicon at 300 K.



The reflectivity of a polished silicon wafer is determined from the complex refractive index.

Absorbing Solar Energy

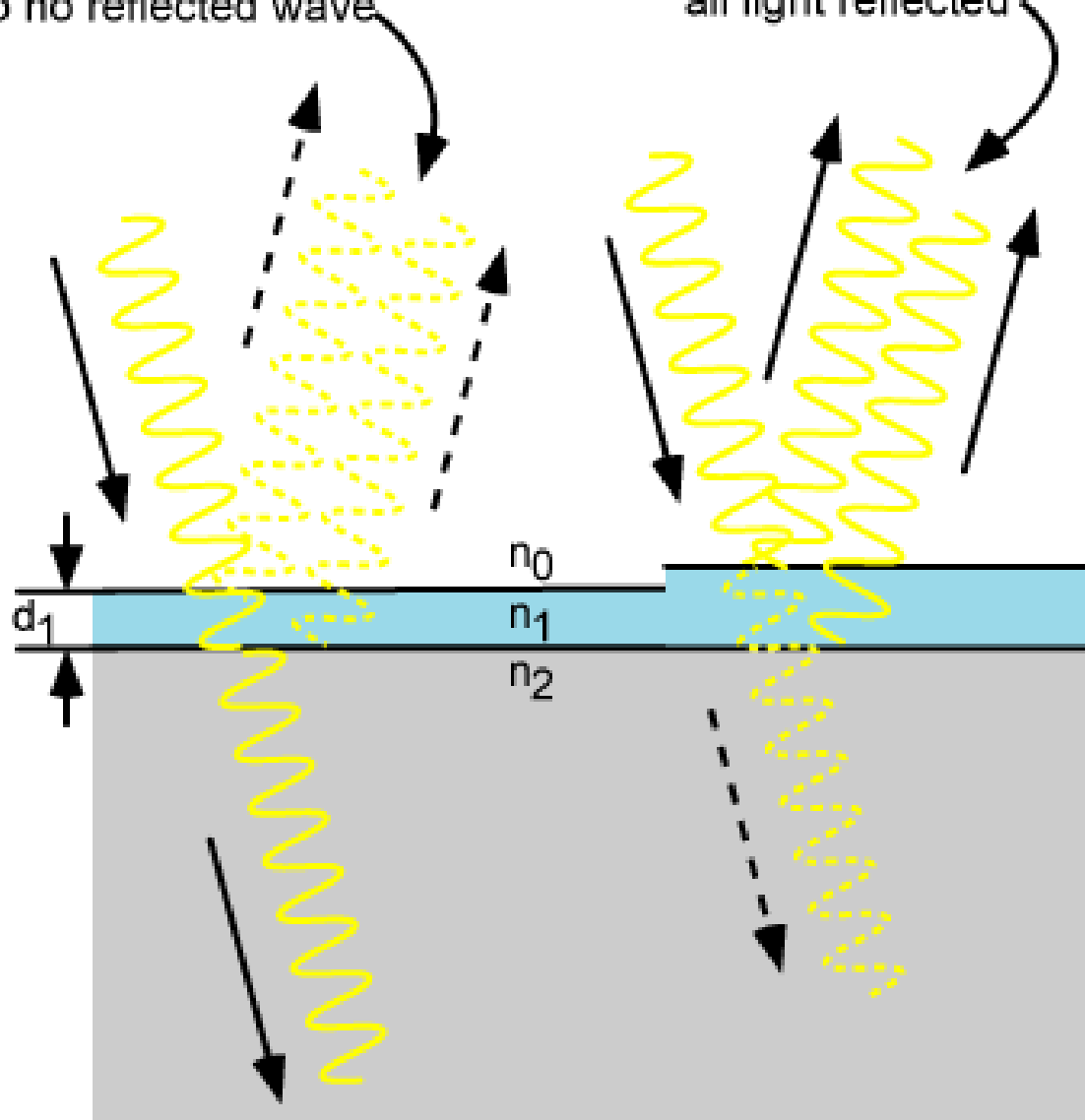
- Optical Properties of Solar Cell Materials -

- **Antireflection Coatings**

Anti-reflection coatings on solar cells are similar to those used on other optical equipment such as camera lenses. They consist of a thin layer of dielectric material, with a specially chosen thickness so that interference effects in the coating cause the wave reflected from the anti-reflection coating top surface to be out of phase with the wave reflected from the semiconductor surfaces. These out-of-phase reflected waves destructively interfere with one another, resulting in zero net reflected energy.

(a) destructive interference
so no reflected wave

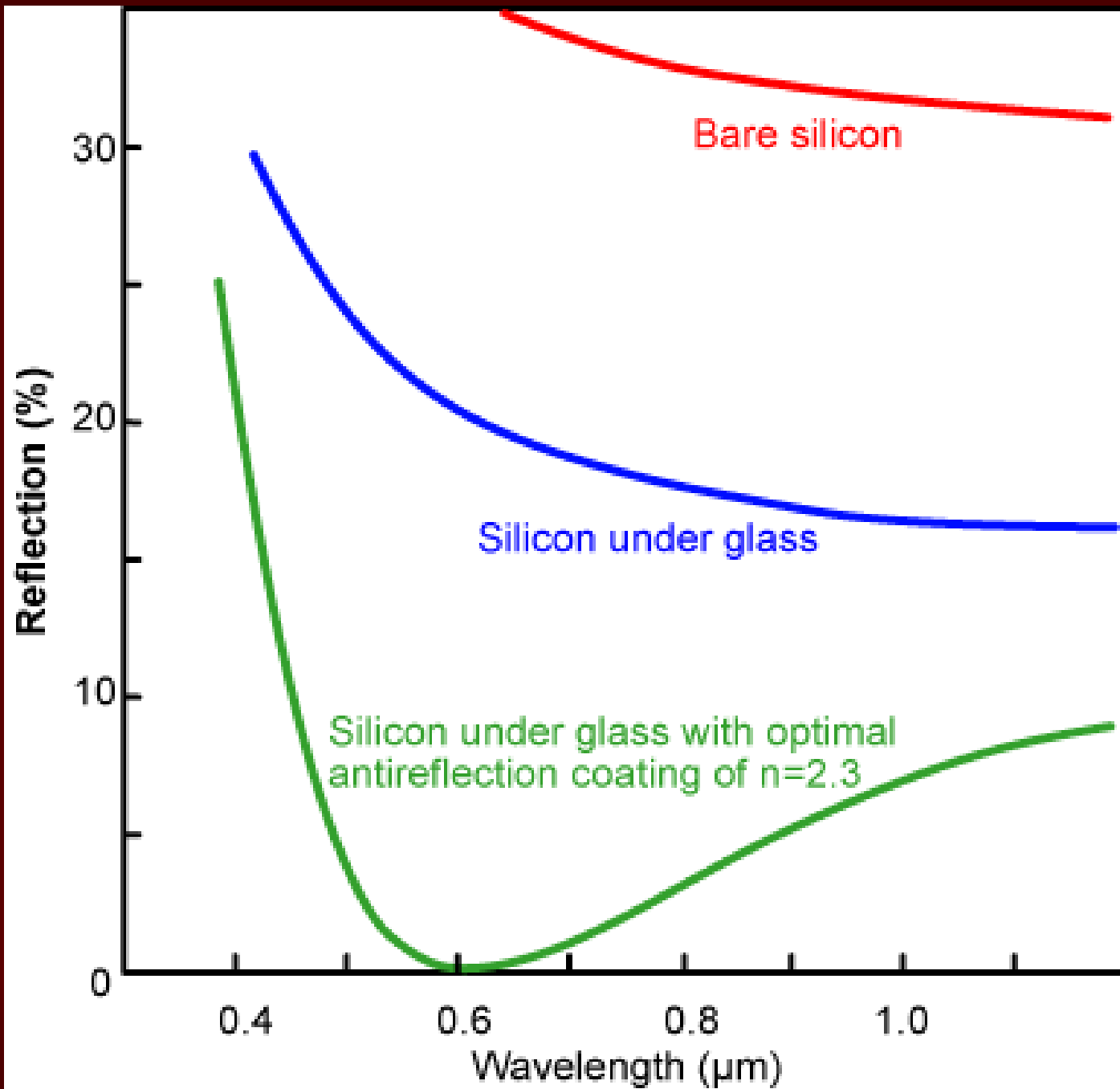
(b) constructive interference so
all light reflected



all light transmitted into
semiconductor

no light transmitted into
semiconductor

$$d_1 = \frac{\lambda_0}{4n_1}$$



Absorbing Solar Energy

- Photoluminescence -

- **Photoluminescence** (abbreviated as **PL**) is a process in which a substance absorbs photons (electromagnetic radiation) and then re-radiates photons.
- Quantum mechanically, this can be described as an excitation to a higher energy state and then a return to a lower energy state accompanied by the emission of a photon.

Absorbing Solar Energy

- Photoluminescence -

- The simplest photoluminescent processes are **resonant radiations**, in which a photon of a particular wavelength is absorbed and an equivalent photon is immediately emitted. This process involves no significant internal energy transitions of the chemical substrate between absorption and emission and is extremely fast, of the order of 10 nanoseconds.
- More interesting processes occur when the chemical substrate undergoes internal energy transitions before re-emitting the energy from the absorption event. The most familiar such effect is **fluorescence**, which is also typically a fast process, but in which some of the original energy is dissipated so that the emitted light photons are of lower energy than those absorbed. The generated photon in this case is said to be red shifted, referring to the loss of energy as **Jablonski diagram** shows.

Absorbing Solar Energy

- Photoluminescence -

- **Luminescence** spontaneous emission in solids
- **Fluorescence** fast luminescence
electric-dipole allowed, $\tau_R \sim \text{ns}$
- **Phosphorescence** slow luminescence
electric-dipole forbidden, $\tau_R \sim \mu\text{s} - \text{ms}$
- **Electroluminescence** electrical excitation
- **Photoluminescence** optical excitation
- **Cathodoluminescence** cathode ray (e-beam) excitation

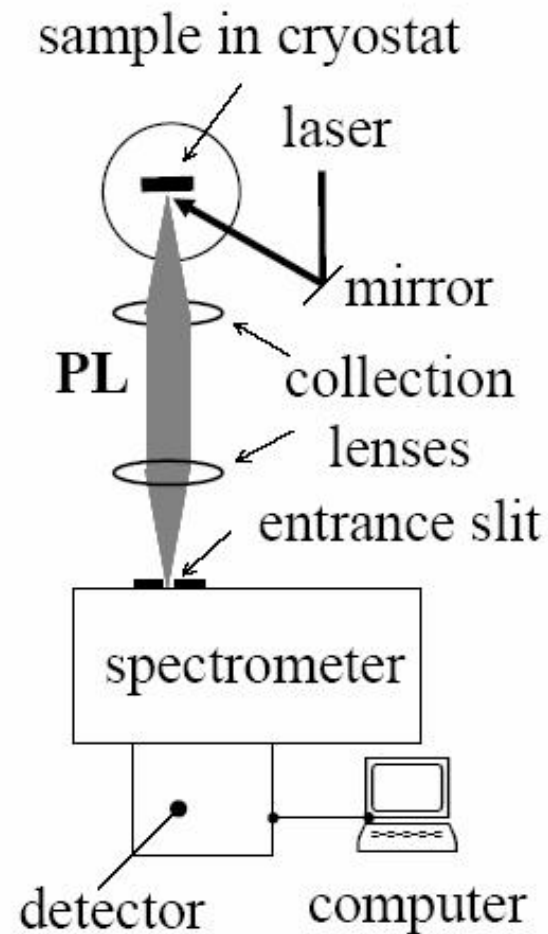
Absorbing Solar Energy

- Photoluminescence -

- Photoluminescence is an important technique for measuring the purity and crystalline quality of semiconductors such as GaAs and InP. Several variations of photoluminescence exist, including photoluminescence excitation (PLE).
- Time-resolved photoluminescence (TRPL) is a method where the sample is excited with a light pulse and then the decay in photoluminescence with respect to time is measured. This technique is useful in measuring the minority carrier lifetime of III-V semiconductors like Gallium arsenide (GaAs).

Absorbing Solar Energy

- Photoluminescence -



Photoluminescence (PL) spectroscopy

- fixed frequency laser, measure spectrum by scanning spectrometer

PL excitation spectroscopy (PLE)

- detect at peak emission, vary laser frequency
- effectively measures absorption

Time-resolved PL spectroscopy

- short pulse laser + fast detector
- measure lifetimes, relaxation processes

Solar Cell Equations

- PV Device -

A solid-state electrical device that converts light directly into direct current electricity of voltage-current characteristics that are a function of the characteristics of the light source and the materials in and design of the device. Solar photovoltaic devices are made of various semiconductor materials including silicon, cadmium sulfide, cadmium telluride, and gallium arsenide, and in single crystalline, multicrystalline, or amorphous forms.

Basic equations to solve are:

$$\nabla \cdot \epsilon \nabla V = -(p - n + N_D^+ - N_A^-)$$

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + U_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + U_p$$

$$J_n = qn(x)\mu_n E(x) + qD_n \frac{dn}{dx}$$

$$J_p = qp(x)\mu_p E(x) - qD_p \frac{dp}{dx}$$

S. Selberherr: "Analysis and Simulation of Semiconductor Devices", Springer, 1984.

Solar Cell Equations

- Important Generation-Recombination Mechanisms -

- Auger GR mechanism (high carrier concentrations)
- SRH GR mechanism
- Surface SRH GR mechanism
- Optical recombination
- Optical Generation

GR Mechanisms

Photons and phonons (review):

- **Photons** → quantum of energy in an electromagnetic wave

$$E = hf \approx (1 - 4) eV$$

$$p = h/\lambda, \quad \lambda = c/f \approx 0.4 \mu m \quad (E = 1 eV)$$

↓

large energy, small momentum

- **Phonons** → quantum of energy in an elastic wave

$$E = hf \approx (0.02 - 0.06) eV$$

$$p = h/\lambda, \quad \lambda = v_s/f \approx 1.8 nm$$

$$(E = 0.02 eV, v_s = 8.5 \times 10^3 m/s)$$

↓

small energy, large momentum

Generation-Recombination mechanisms:

Notation:

$g \rightarrow$ generation rate

$r \rightarrow$ recombination rate

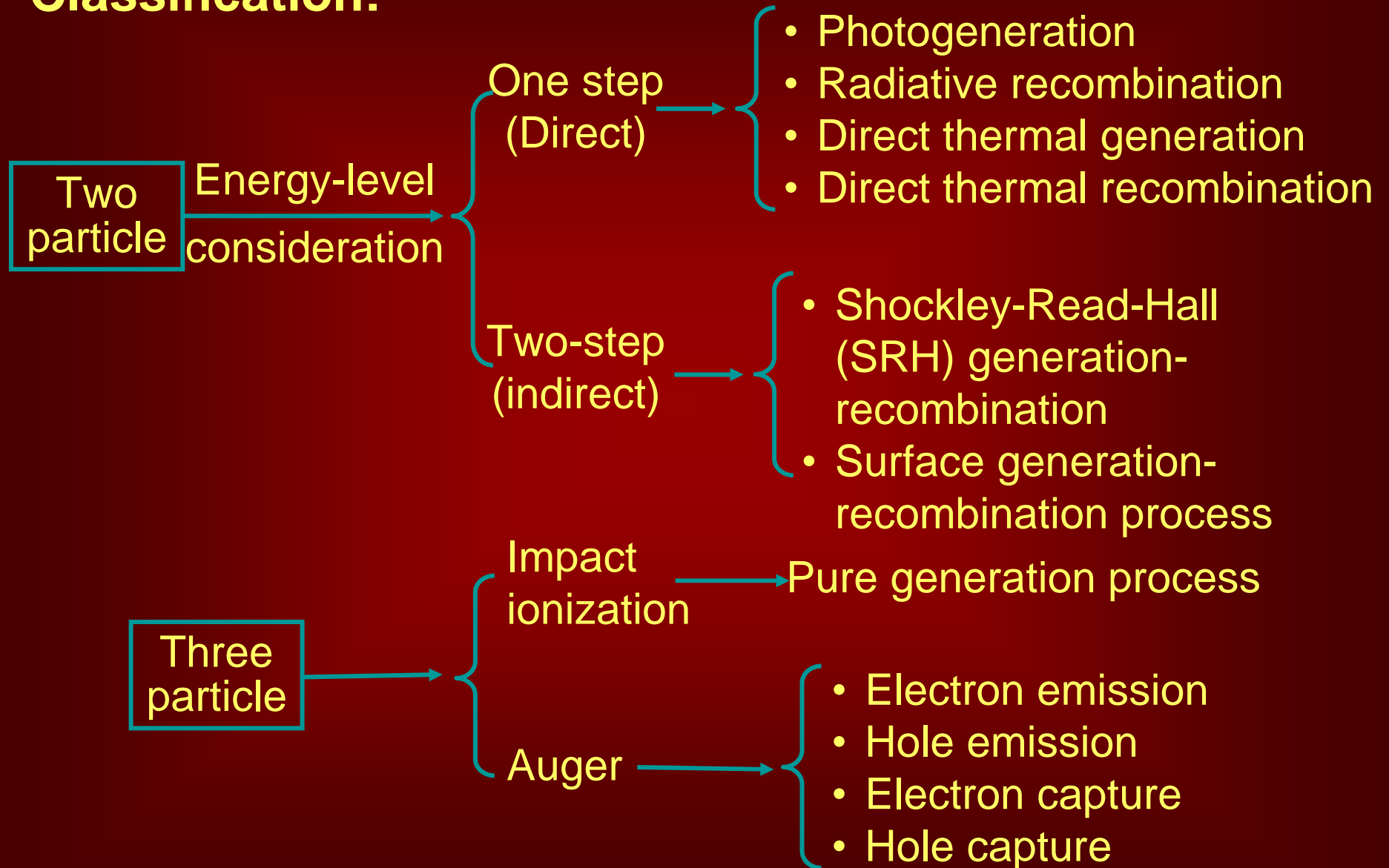
$R = r - g \rightarrow$ net recombination rate

Importance:

Diodes, BJTs \rightarrow R plays a crucial role in the operation of the device

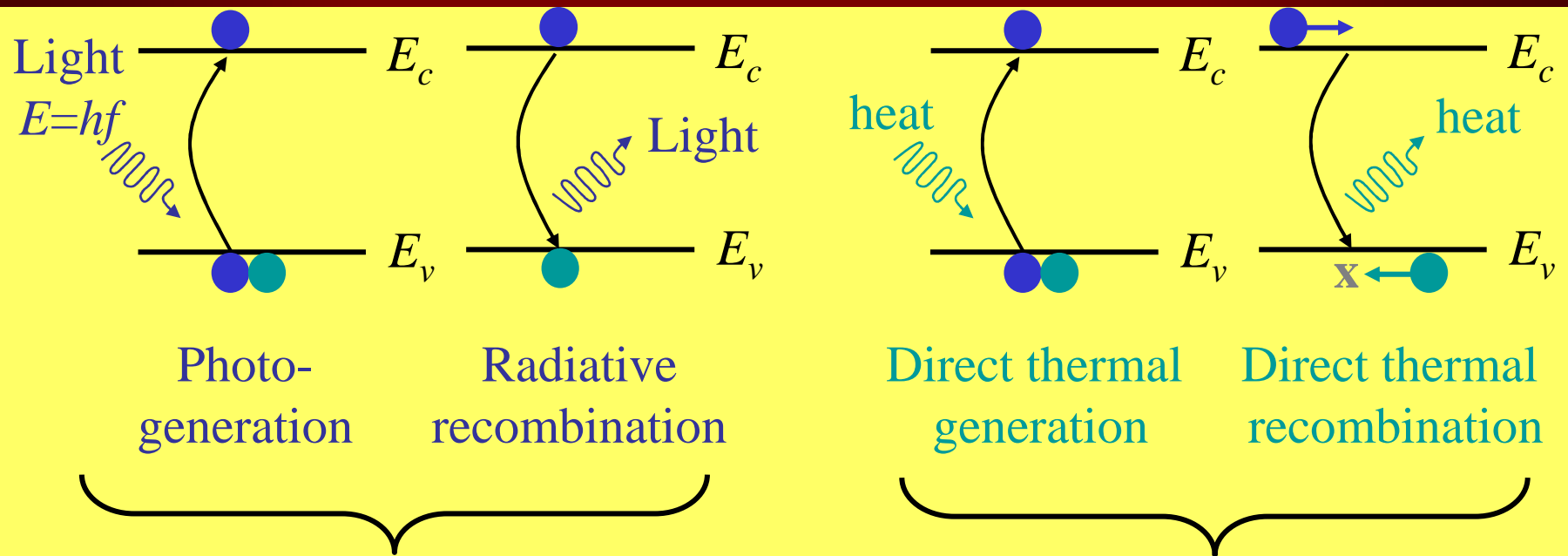
Unipolar devices (MOSFET's, MESFETs, Schottky diodes) \rightarrow No influence except when investigating high-field and breakdown phenomena

Classification:



(1) Direct processes

Diagrammatic description:

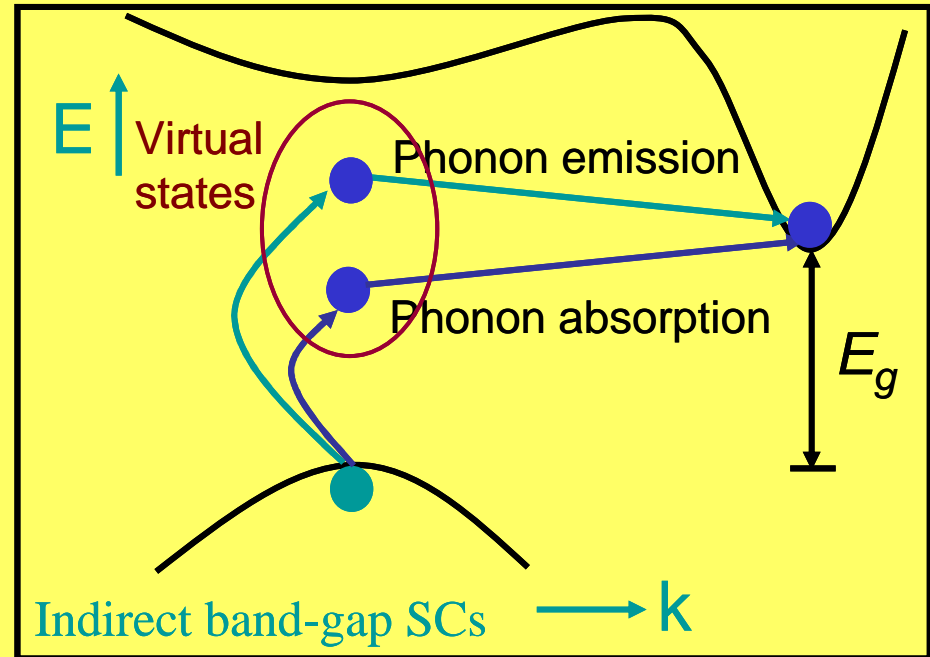
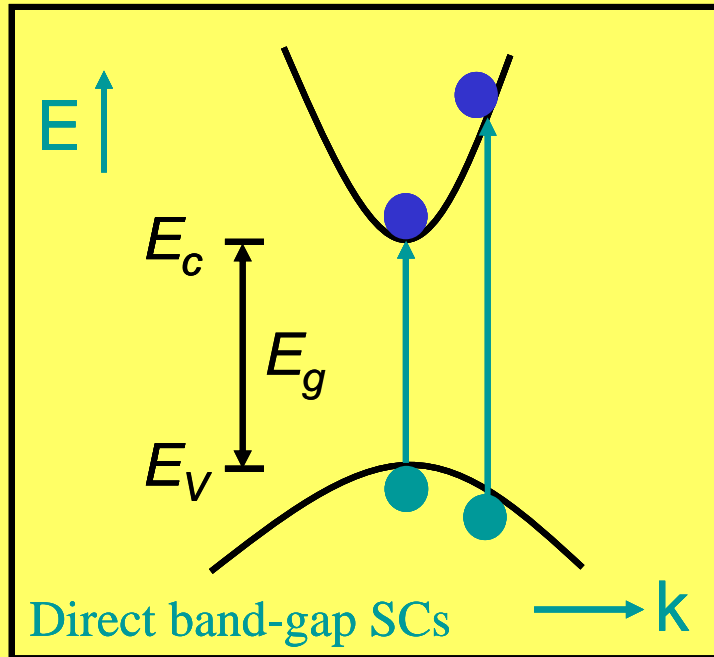


Important for:

- narrow-gap semiconductors
- direct band-gap SCs used for fabricating LEDs for optical communications

Not the usual means by which the carriers are generated or recombine

- Photogeneration → band-diagrammatic description:



Momentum and energy conservation:

$$\begin{aligned}
 p_f &= p_i \\
 E_f &= E_i + E_{ph}
 \end{aligned}$$

final ← initial → photon

$$\begin{aligned}
 p_f &= p_i \mp p_s \\
 E_f &= E_i \mp E_s + E_{ph}
 \end{aligned}$$

initial ← phonon → photon

Near the absorption edge, the absorption coefficient can be expressed as:

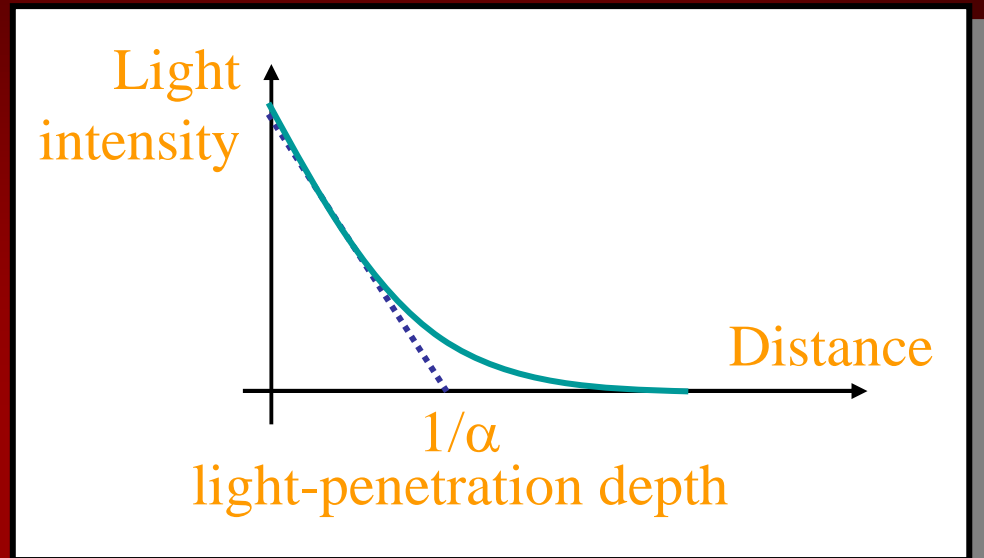
$$\alpha \propto (hf - E_g)^\gamma$$

hf = photon energy

E_g = bandgap

γ = constant

- $\gamma=1/2$ and $1/3$ for allowed direct transitions and forbidden direct transitions
- $\gamma=2$ for indirect transitions where phonons are involved



- Photogeneration-radiative recombination → mathematical description

- Both types of carriers are involved in the process

$$r = Bpn, \quad g = Bp_0n_0 = Bn_i^2 \Rightarrow \mathbf{B} = \text{optical capture/emission rate}$$

$$R = r - g = B(pn - n_i^2) \rightarrow p = p_0 + \Delta p, \quad n = n_0 + \Delta n$$

$$R = B \cdot \Delta n (p_0 + n_0 + \Delta n)$$

$$\begin{cases} B(\text{GaAs}) = (1.3 \pm 0.3) \times 10^{-10} \text{ cm}^3 / \text{s} \\ B(\text{Si}) = 2 \times 10^{-15} \text{ cm}^3 / \text{s} \end{cases}$$

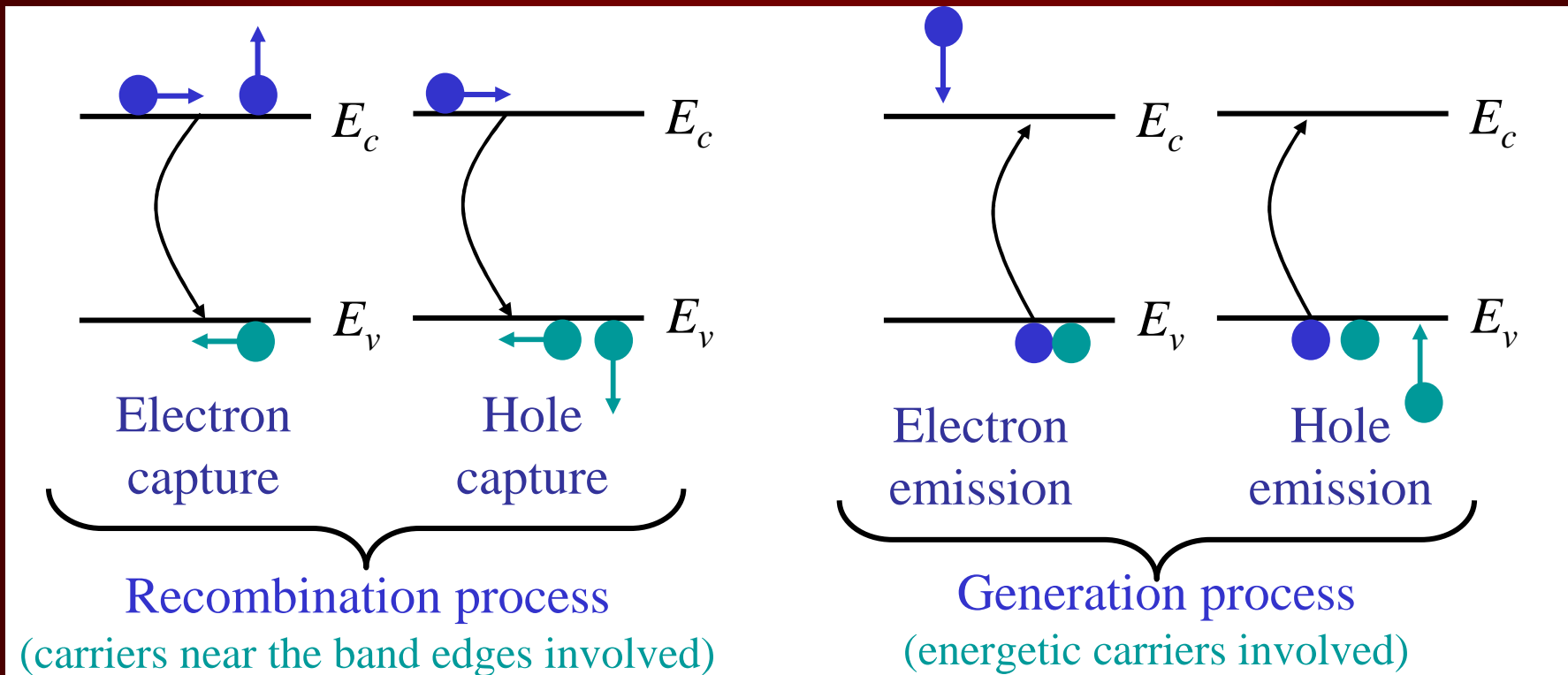
- Limiting cases:

$$\text{(a) Low-level injection: } \Delta n, n_0 \ll p_0 \rightarrow \tau_{rad} = \frac{\Delta n}{R} \approx \frac{1}{Bp_0}$$

$$\text{(b) High-level injection: } \Delta n \gg n_0, p_0 \rightarrow \tau_{rad} = \frac{\Delta n}{R} \approx \frac{1}{B\Delta n}$$

(2) Auger processes:

Diagrammatic description



- **Auger generation** takes place in regions with high concentration of mobile carriers with **negligible current flow**
- **Impact ionization** requires **non-negligible current flow**

- Auger process → mathematical description

- Three carriers are involved in the process

$$r = C_n p n^2 + C_p p^2 n, \quad g = C_n p_0 n_0^2 + C_p p_0^2 n_0$$

$$R = r - g = C_n (p n^2 - p_0 n_0^2) + C_p (p^2 n - p_0^2 n_0)$$

↓

$$p = p_0 + \Delta p, \quad n = n_0 + \Delta n$$

$$\tau_{Auger} = \frac{\Delta n}{R} = \frac{1}{aC_p + bC_n} \rightarrow \begin{cases} a = p_0^2 + 2n_0 p_0 + \Delta n(2p_0 + n_0 + \Delta n) \\ b = n_0^2 + 2n_0 p_0 + \Delta n(2n_0 + p_0 + \Delta n) \end{cases}$$

- Limiting cases (*p*-type sample):

(a) Low-level injection: $\tau_{Auger} = [C_p p_0^2 + C_n p_0(2n_0 + \Delta n)]^{-1}$

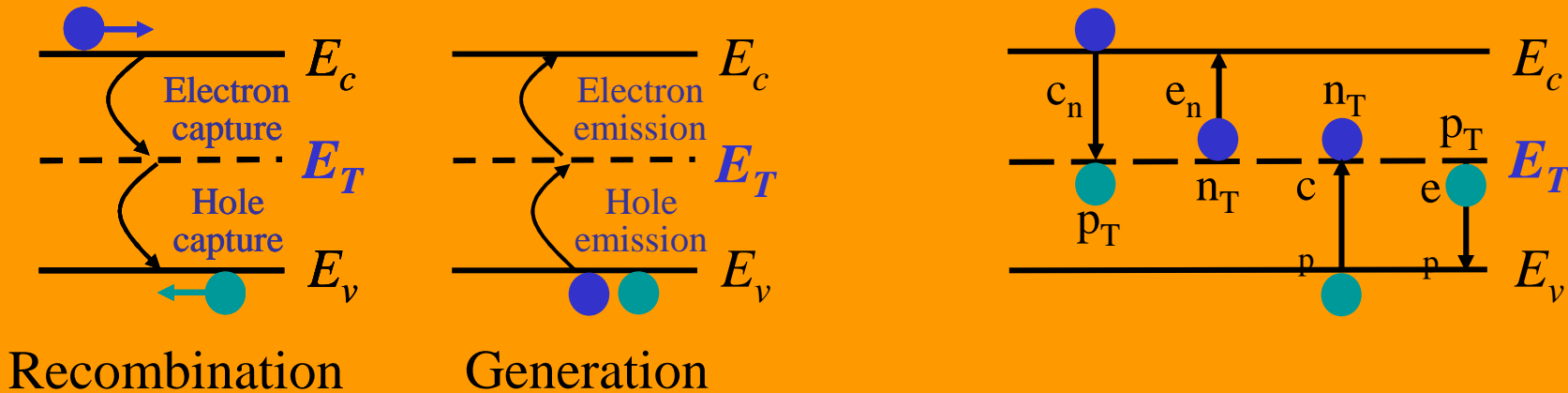
(b) High-level injection: $\tau_{Auger} = [\Delta n^2 (C_p + C_n)]^{-1}$

- Auger Coefficients:
(*Silvaco*)

T [K]	C_n [cm⁶/s]	C_p [cm⁶/s]
77	2.3x10 ⁻³¹	7.8x10 ⁻³²
300	2.8x10 ⁻³¹	9.9x10 ⁻³²
400	2.8x10 ⁻³¹	1.2x10 ⁻³¹

(3) Shockley-Read-Hall Mechanism:

Diagrammatic description:



Mathematical model:

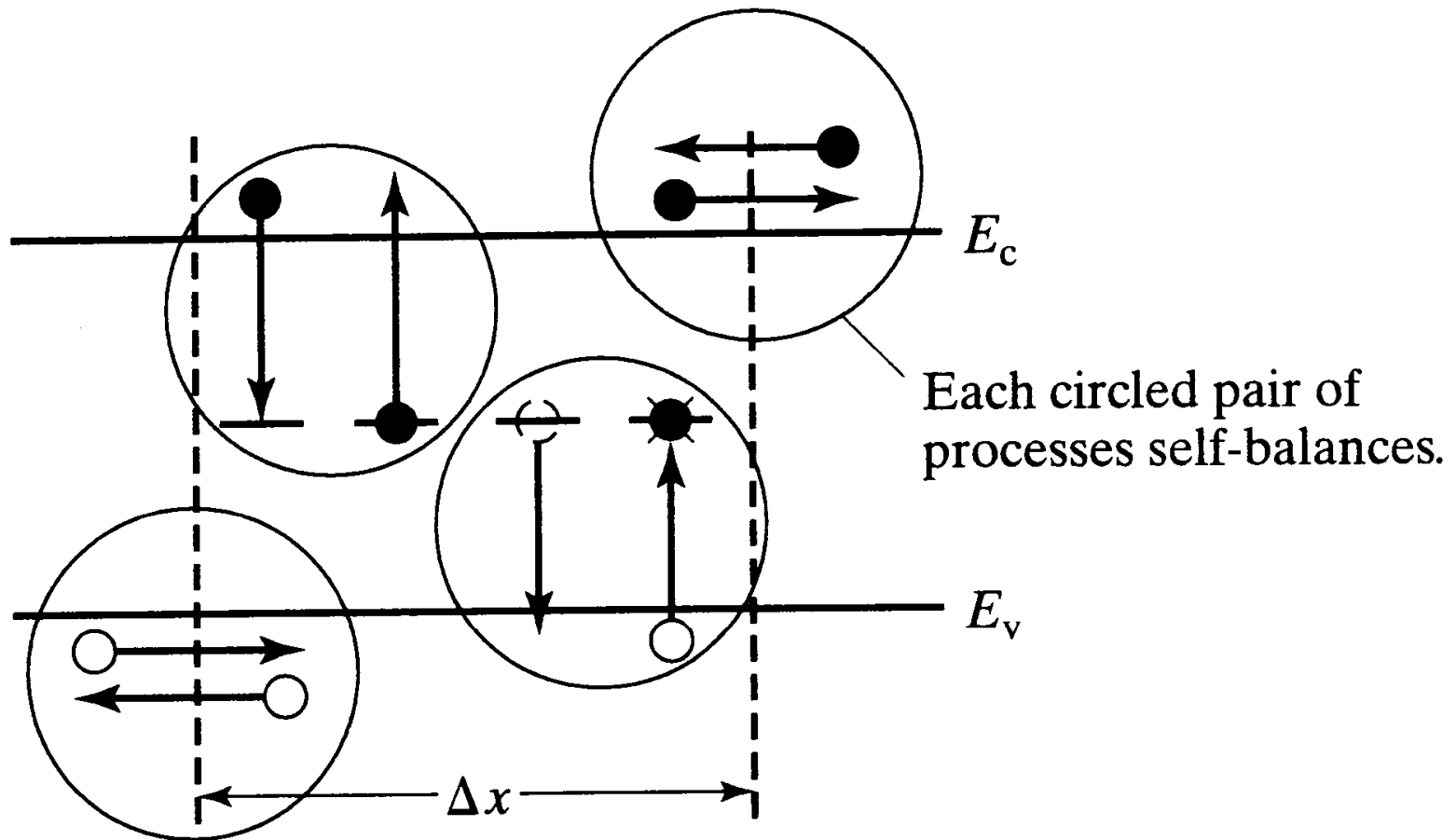
$$\frac{dn}{dt} = e_n n_T - c_n n p_T$$

$$\frac{dp}{dt} = e_p p_T - c_p p n_T$$

Two types of carriers involved in the process

$$\left. \begin{aligned} n_T &= N_T f_T \\ p_T &= N_T (1 - f_T) \end{aligned} \right\} \rightarrow n_T + p_T = N_T$$

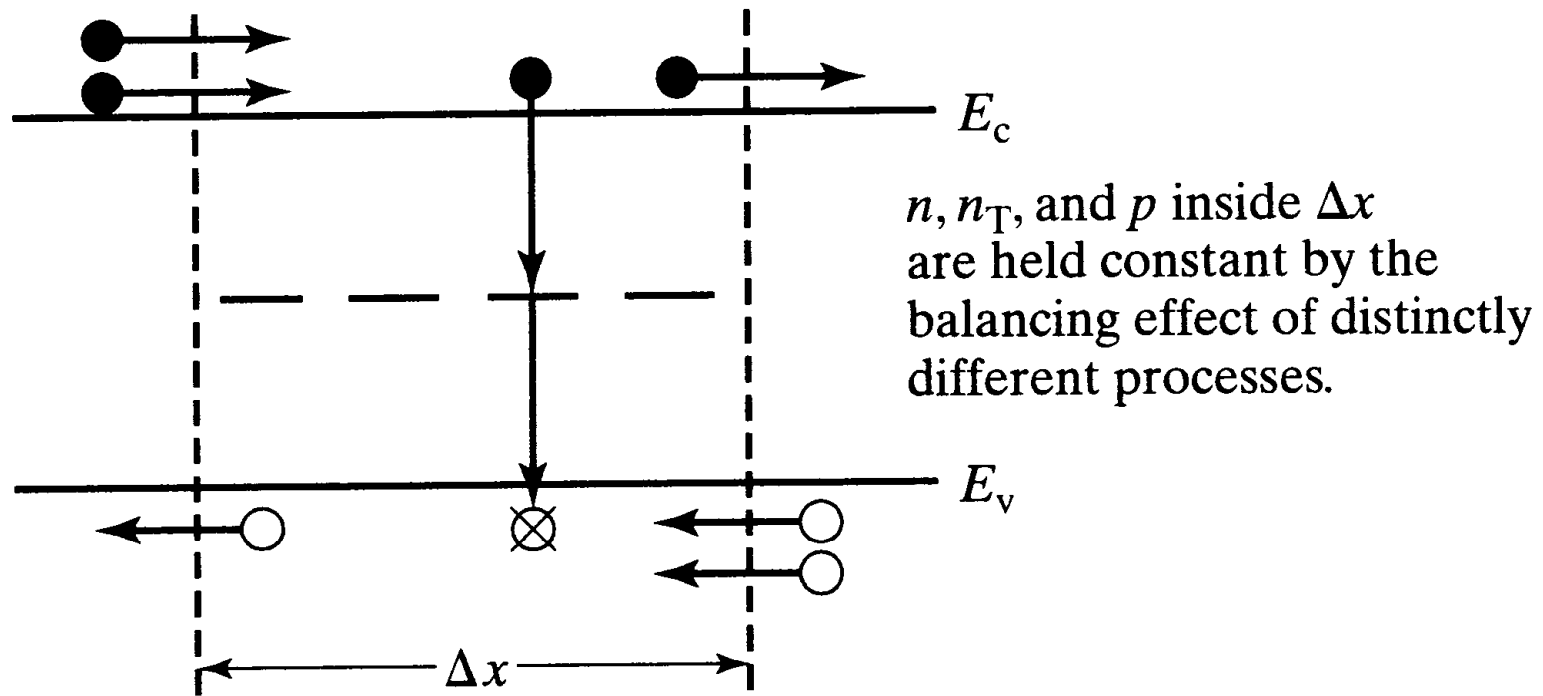
Look at Equilibrium first



(a) Equilibrium

Detailed Balance

Now look at steady-state next



(b) Steady-state

- Thermal equilibrium conditions:

$$dn/dt = 0, dp/dt = 0$$



$$\begin{cases} c_n np_T = e_n n_T \\ e_p p_T = c_p pn_T \end{cases} \Rightarrow \begin{cases} e_n = c_n n_1 \\ e_p = c_p p_1 \end{cases}$$

n_1 and p_1 are the electron and hole densities when $E_F = E_T$

- Steady-state conditions:

$$\begin{cases} R_n = R_{nc} - R_{ne} = c_n np_T - e_n n_T = c_n (np_T - n_1 n_T) \\ R_p = R_{pc} - R_{pe} = c_p pn_T - e_p p_T = c_p (pn_T - p_1 p_T) \end{cases}$$



$$f_T = \frac{c_n n + c_p p_1}{c_n (n + n_1) + c_p (p + p_1)} \rightarrow R = \frac{np - n_i^2}{\frac{1}{c_p N_T} (n + n_1) + \frac{1}{c_n N_T} (p + p_1)}$$

- Define carrier lifetimes:

$$\tau_p = \frac{1}{c_p N_T} = \frac{1}{\sigma_p v_{th} N_T}, \quad \tau_n = \frac{1}{c_n N_T} = \frac{1}{\sigma_n v_{th} N_T}$$

- Empirical expressions for electron and hole lifetimes:

$$\tau_n = \frac{\tau_n^0}{1 + \frac{N_A + N_D}{N_n^{ref}}}, \quad \tau_p = \frac{\tau_p^0}{1 + \frac{N_A + N_D}{N_p^{ref}}}$$

τ_{n0} [s]	N_n^{ref} [cm ⁻³]	τ_{p0} [s]	N_p^{ref} [cm ⁻³]	Source
5×10^{-5}	5×10^{16}	5×10^{-5}	5×10^{16}	D'Avanzo
3.94×10^{-4}	7.1×10^{15}	3.94×10^{-4}	7.1×10^{15}	Dhanasekaran

- Limiting cases:

$$\tau_{SRH} = \frac{\Delta n}{R} = \frac{\tau_p (n_0 + \Delta n + n_1) + \tau_n (p_0 + \Delta n + p_1)}{n_0 + p_0 + \Delta n}$$

(a) Low level injection (*p*-type sample): $\tau_{SRH} = \frac{\Delta n}{R} = \tau_n$

(b) High-level injection: $\tau_{SRH} = \frac{\Delta n}{R} = \tau_n + \tau_p$

- Generation process ($p \cong n \cong 0$):

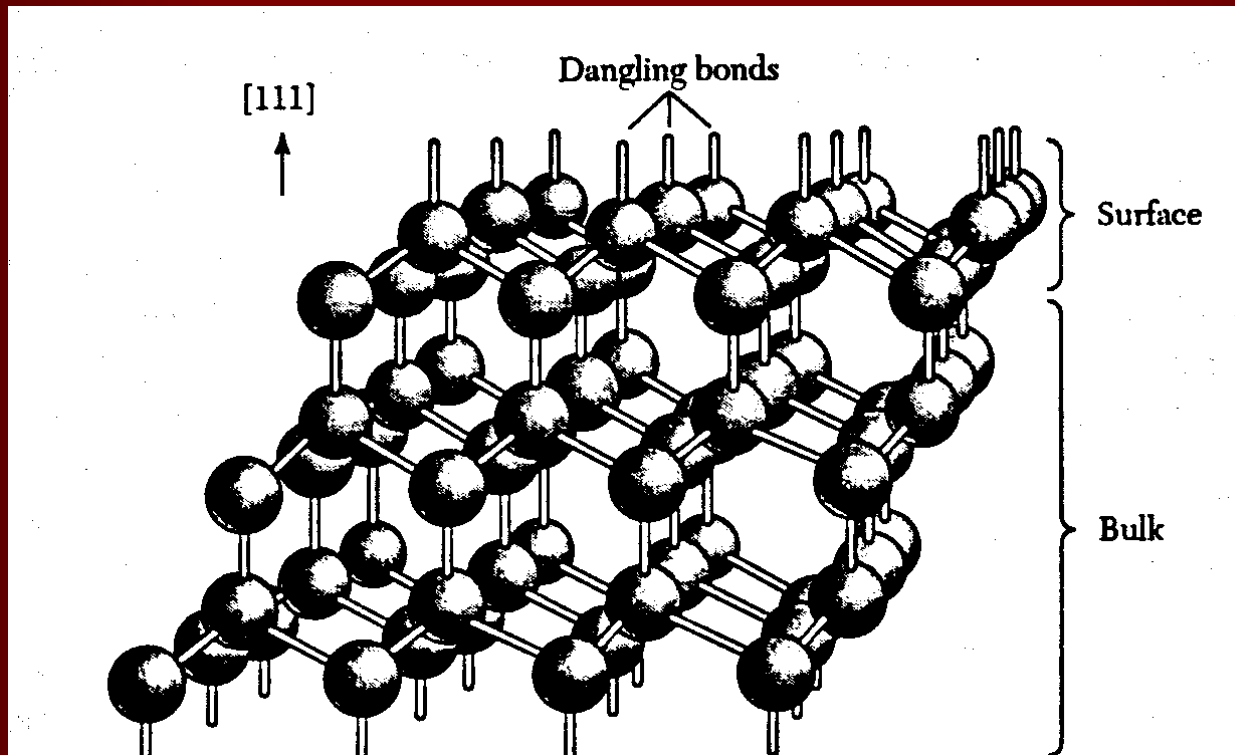
$$R = \frac{-n_i^2}{\tau_p n_1 + \tau_n p_1} = -G \rightarrow G = \frac{n_i}{\tau_g}$$

$$\tau_g = \text{generation rate} \Rightarrow \tau_g = \tau_p e^{\alpha} + \tau_n e^{-\alpha}, \quad \alpha = \frac{E_T - E_i}{k_B T}$$

Typical #'s

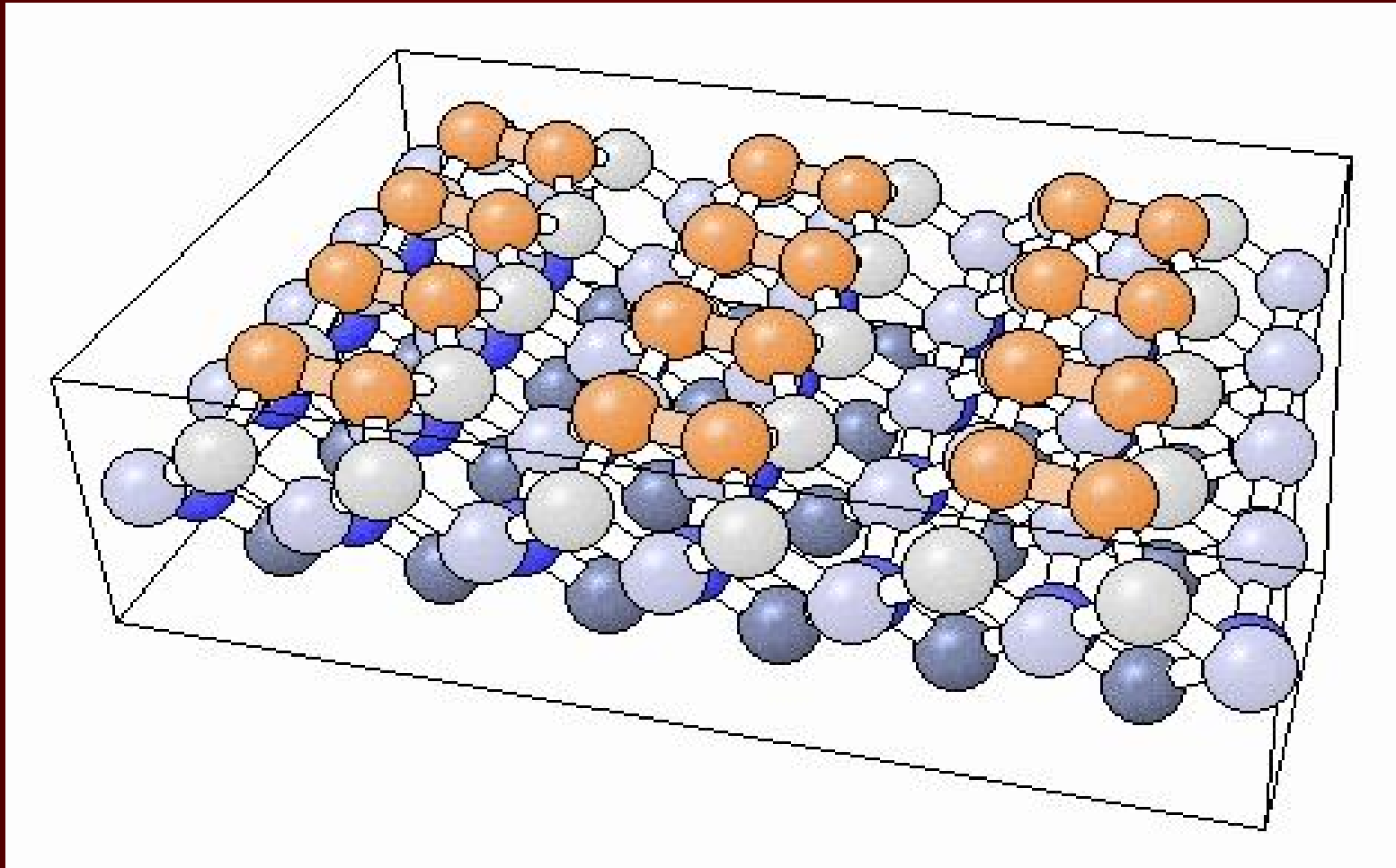
	N_T	E_T	S_{TN}	S_{TP}	S_N	S_P
Material	[cm ⁻³]	[eV]	[m ²]	[m ²]	[m/s]	[m/s]
Si, Ge	1e13	0.0	1e-15	1e-15	0.0	0.0
III-Vs	2e16	0.4	1e-14	1e-13	0.0	0.0

3a. Surface Recombination



Lattice periodicity broken at surface/interface - mid-gap E levels
Carriers generated-recombined per unit area

Surface States



Reconstruction

- Processes and descriptions analogous to bulk R-G using surface parameters
- For a **single energy level** surface state:

$$\begin{array}{l}
 r_N = c_n (p_T n - n_T n_1) \\
 r_P = c_p (n_T p - p_T p_1)
 \end{array}
 \longrightarrow
 \begin{array}{l}
 r_{Ns} = c_{ns} (p_{Ts} n_s - n_{Ts} n_{1s}) \\
 r_{Ps} = c_{ps} (n_{sT} p_s - p_{Ts} p_{1s})
 \end{array}$$

$$n_1 = n_i e^{(E_T - E_i)/kT}$$

$$p_1 = p_i e^{(E_i - E_T)/kT}$$

$$n_{1s} = n_i e^{(E_{Ts} - E_i)/kT}$$

$$p_{1s} = p_i e^{(E_i - E_{Ts})/kT}$$

$$R = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)}$$

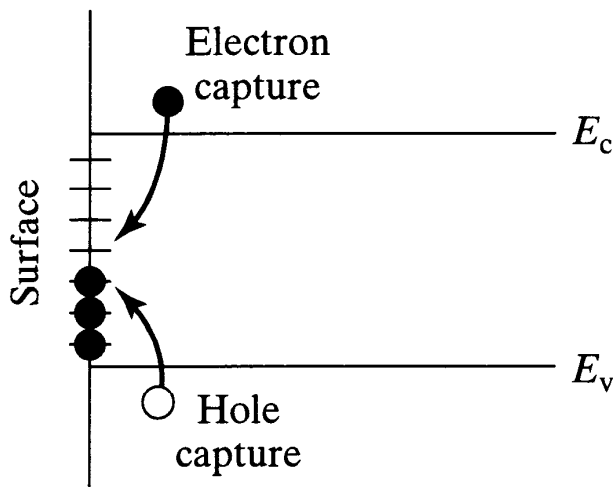
$$R = \frac{n_s p_s - n_i^2}{\frac{1}{s_p}(n_s + n_{1s}) + \frac{1}{s_n}(p_s + p_{1s})}$$

Multi-Level (more realistic)

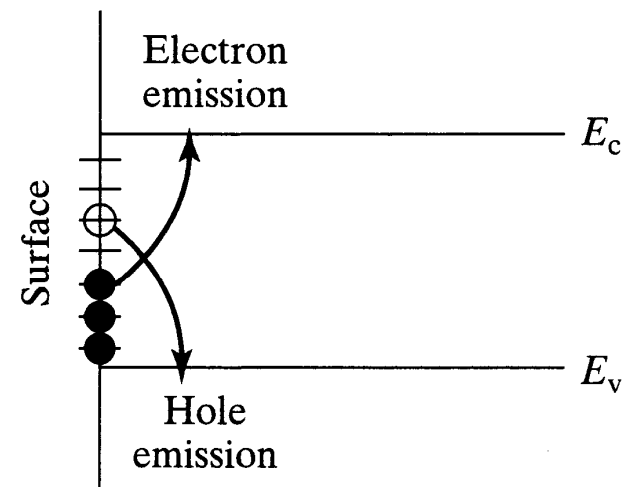
$D_{IT}(E)$ - density of interface traps (per unit area-energy)

$D_{IT}(E)dE$ - density of IT between E and $E+dE$ (replaces N_{T_s})

$$R = \int_{E_v}^{E_c} \frac{n_s p_s - n_i^2}{\frac{1}{c_{ps}} (n_s + n_{1s}) + \frac{1}{c_{ns}} (p_s + p_{1s})} D_{IT}(E) dE$$



(a) Capture



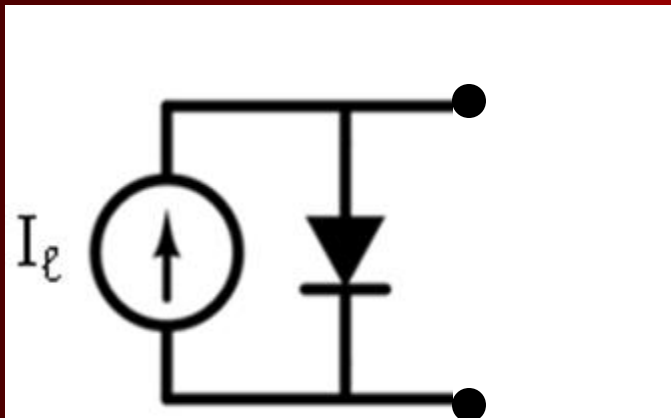
(b) Emission

Solar Cell Equations

- Analytical Model -

- Equations analytical

$$I = I_{\text{ph}} - I_{\text{s}} \left(e^{V/V_{\text{T}}} - 1 \right)$$



Open Circuit:

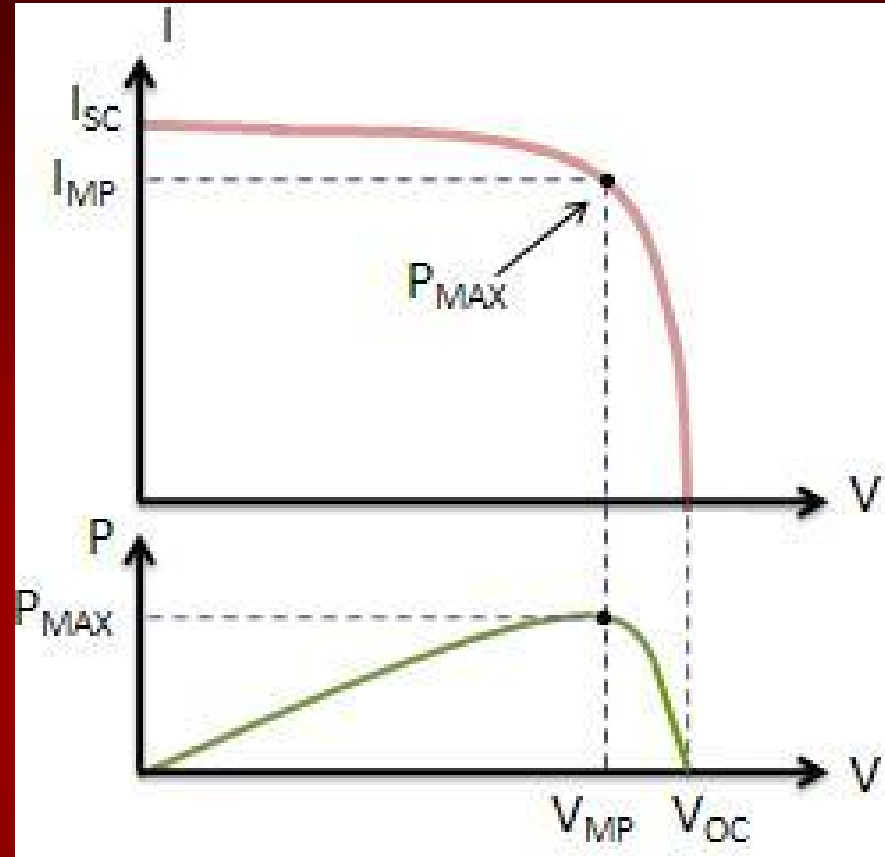
$$I = 0, V = V_{\text{oc}}$$

Short Circuit:

$$V = 0, I = I_{\text{sc}}$$

Open Circuit:
 $I = 0, V = V_{OC}$

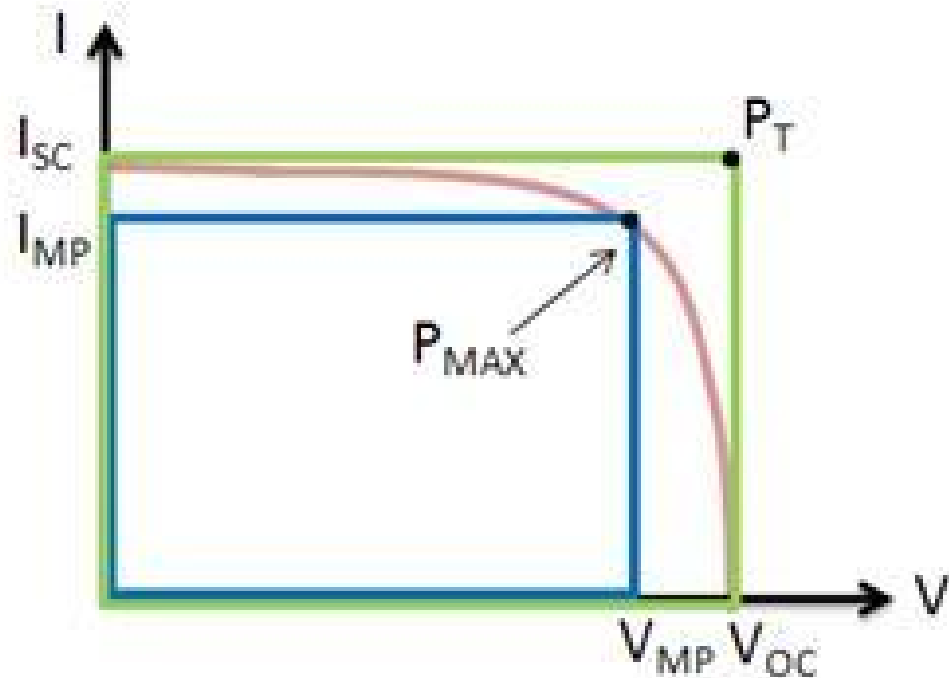
Short Circuit:
 $V = 0, I = I_{SC}$



The power produced by the cell in Watts can be easily calculated along the I-V sweep by the equation $P=IV$. At the I_{SC} and V_{OC} points, the power will be zero and the maximum value for power will occur between the two. The voltage and current at this maximum power point are denoted as V_{MP} and I_{MP} respectively.

The Fill Factor (FF) is essentially a measure of quality of the solar cell. It is calculated by comparing the maximum power to the theoretical power (P_T) that would be output at both the open circuit voltage and short circuit current together. FF can also be interpreted graphically as the ratio of the rectangular areas shown in the figure below.

$$FF = \frac{P_{MAX}}{P_T} = \frac{I_{MP} \cdot V_{MP}}{I_{SC} \cdot V_{OC}}$$



Efficiency is the ratio of the electrical power output P_{out} , compared to the solar power input, P_{in} , into the PV cell. P_{out} can be taken to be P_{MAX} since the solar cell can be operated up to its maximum power output to get the maximum efficiency.

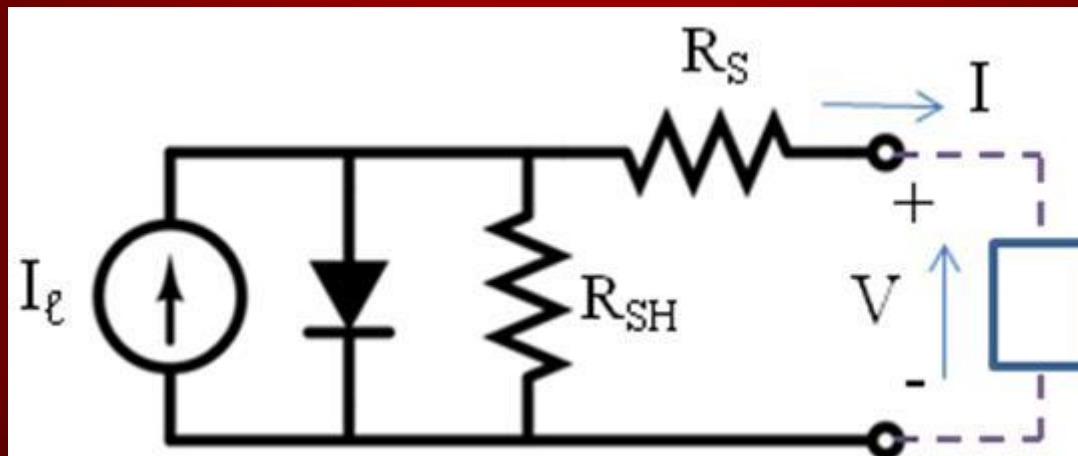
$$\eta = \frac{P_{out}}{P_{in}} \Rightarrow \eta_{MAX} = \frac{P_{MAX}}{P_{in}}$$

P_{in} is taken as the product of the irradiance of the incident light, measured in W/m^2 or in suns ($1000 W/m^2$), with the surface area of the solar cell [m^2]. The maximum efficiency (η_{MAX}) found from a light test is not only an indication of the performance of the device under test, but, like all of the I-V parameters, can also be affected by ambient conditions such as temperature and the intensity and spectrum of the incident light. For this reason, it is recommended to test and compare PV cells using similar lighting and temperature conditions.

During operation, the efficiency of solar cells is reduced by the dissipation of power across internal resistances. These parasitic resistances can be modeled as a parallel shunt resistance (R_{SH}) and series resistance (R_S).

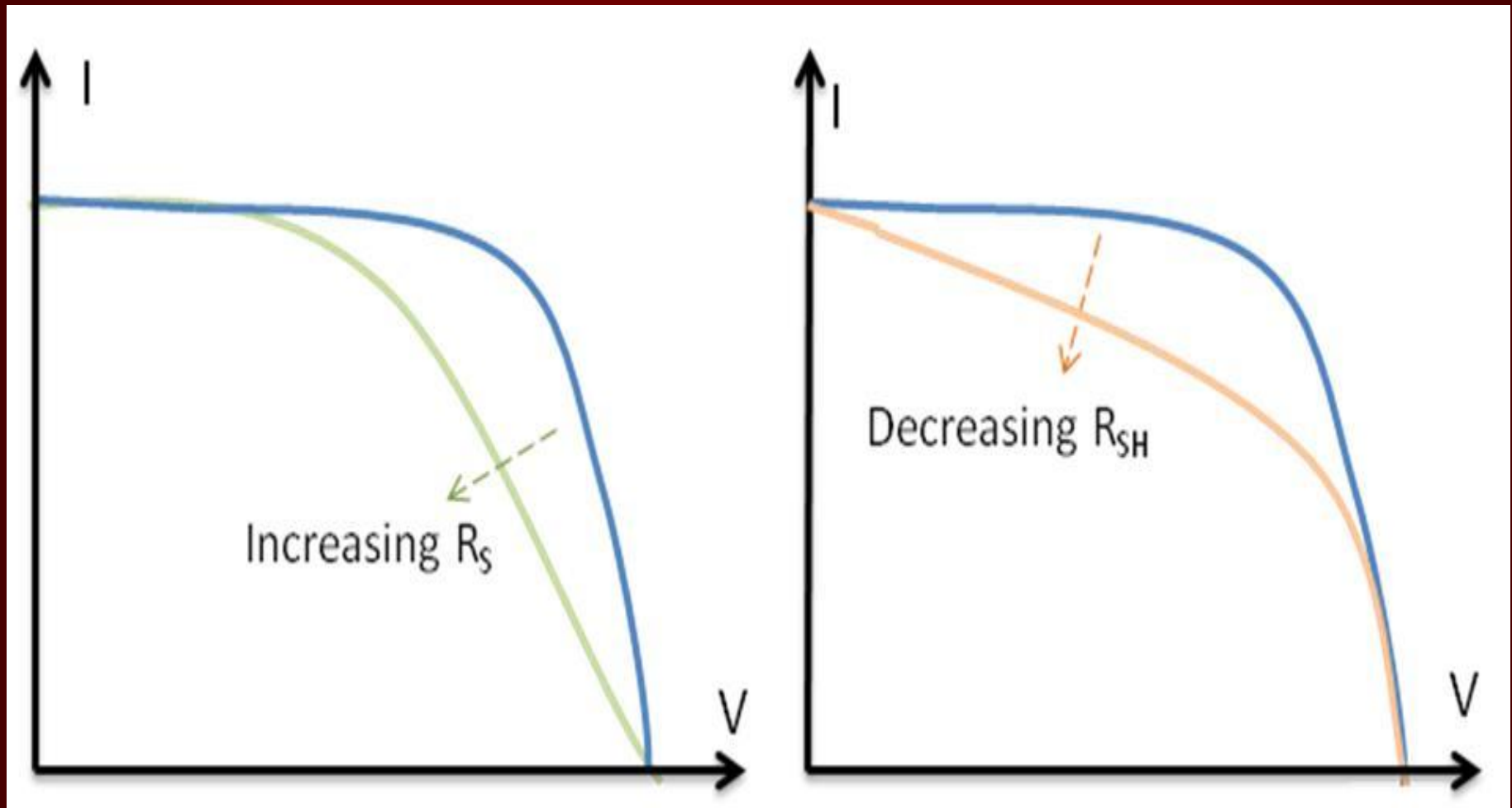
For an ideal cell, R_{SH} would be infinite and would not provide an alternate path for current to flow, while R_S would be zero, resulting in no further voltage drop before the load.

Decreasing R_{SH} and increasing R_S will decrease the fill factor (FF) and P_{MAX} as shown in the figure on the next slide. If R_{SH} is decreased too much, V_{OC} will drop, while increasing R_S excessively can cause I_{SC} to drop instead.

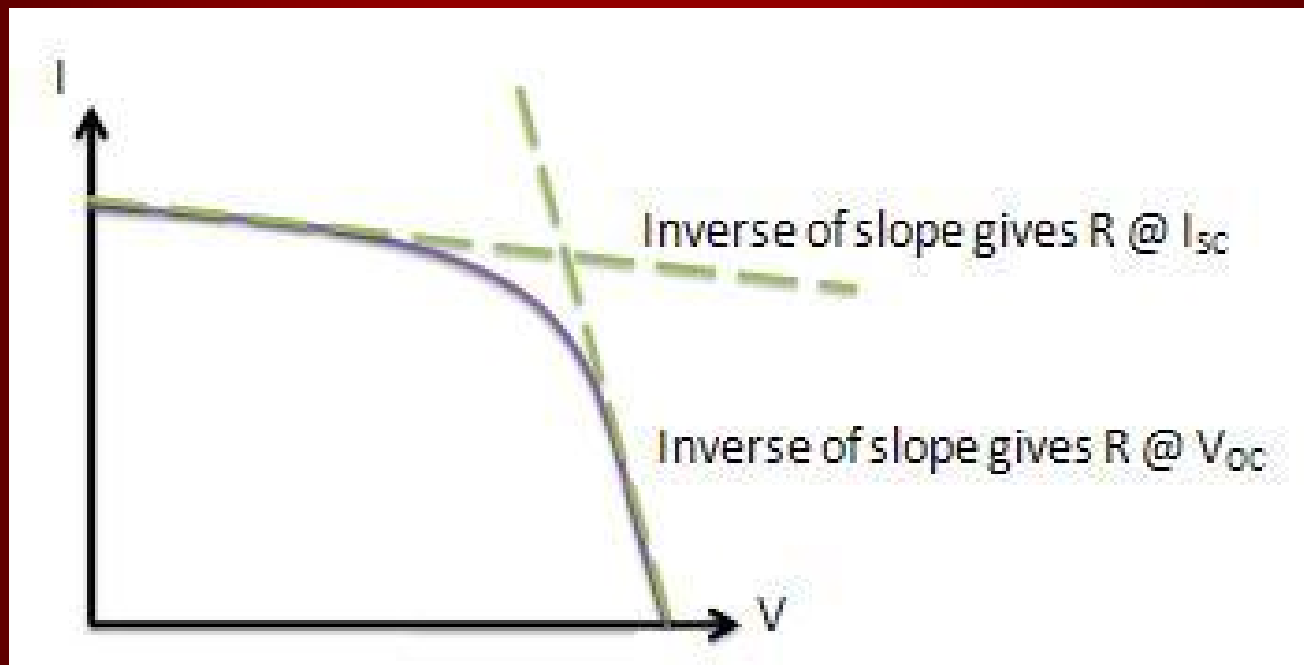


$$I = I_l - I_0 \left(\exp \frac{q(V + I \cdot R_S)}{n \cdot k \cdot T} - 1 \right) - \frac{V + I \cdot R_S}{R_{SH}}$$

Decrease in the FF due to R_S and R_{SH} .

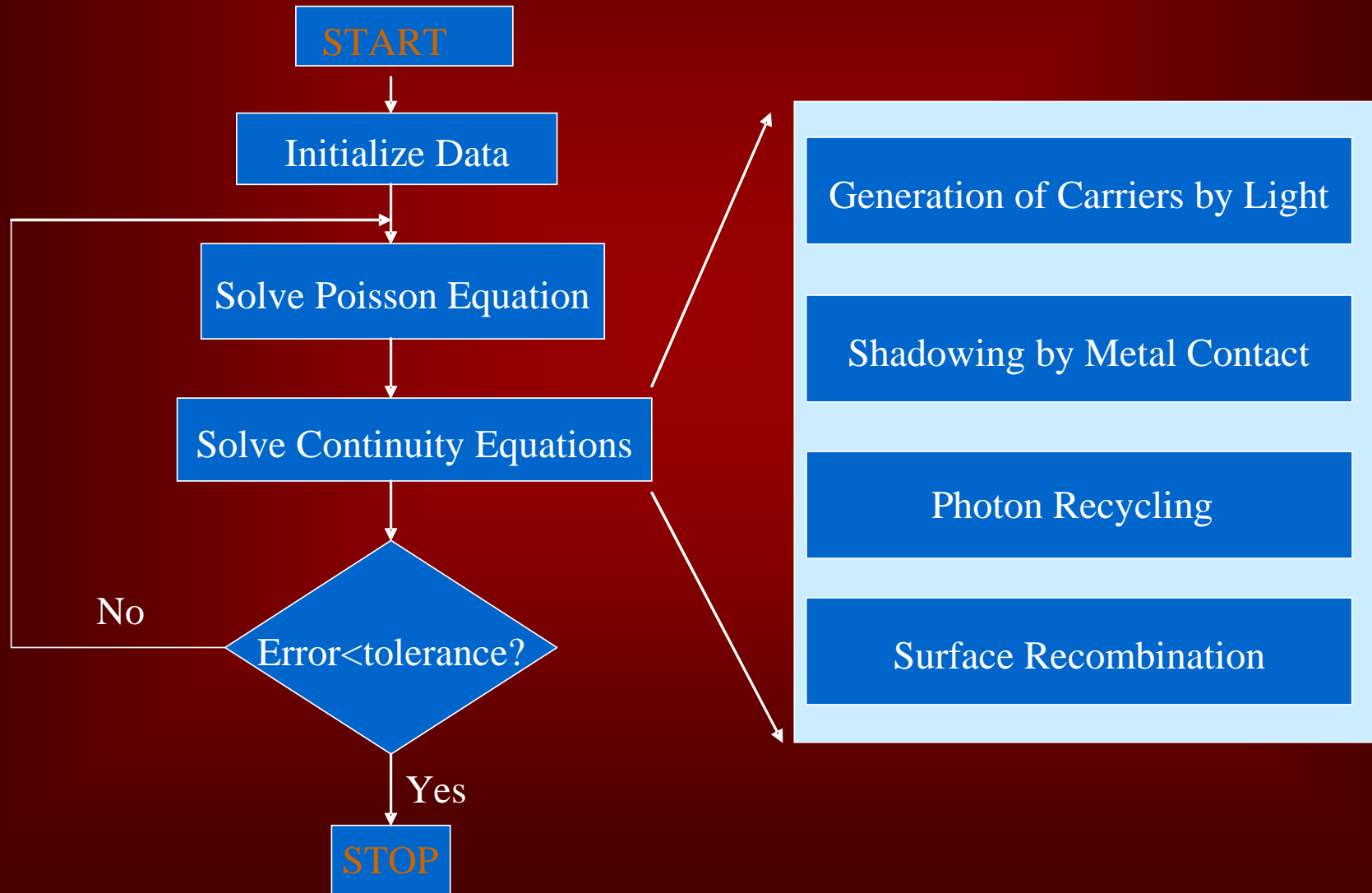


It is possible to approximate the series and shunt resistances, R_S and R_{SH} , from the slopes of the I-V curve at V_{OC} and I_{SC} , respectively. The resistance at V_{oc} , however, is at best proportional to the series resistance but it is larger than the series resistance. R_{SH} is represented by the slope at I_{SC} . Typically, the resistances at I_{SC} and at V_{OC} will be measured and noted.



Solar Cell Eq. Numerical Solution

- Solution Procedure -

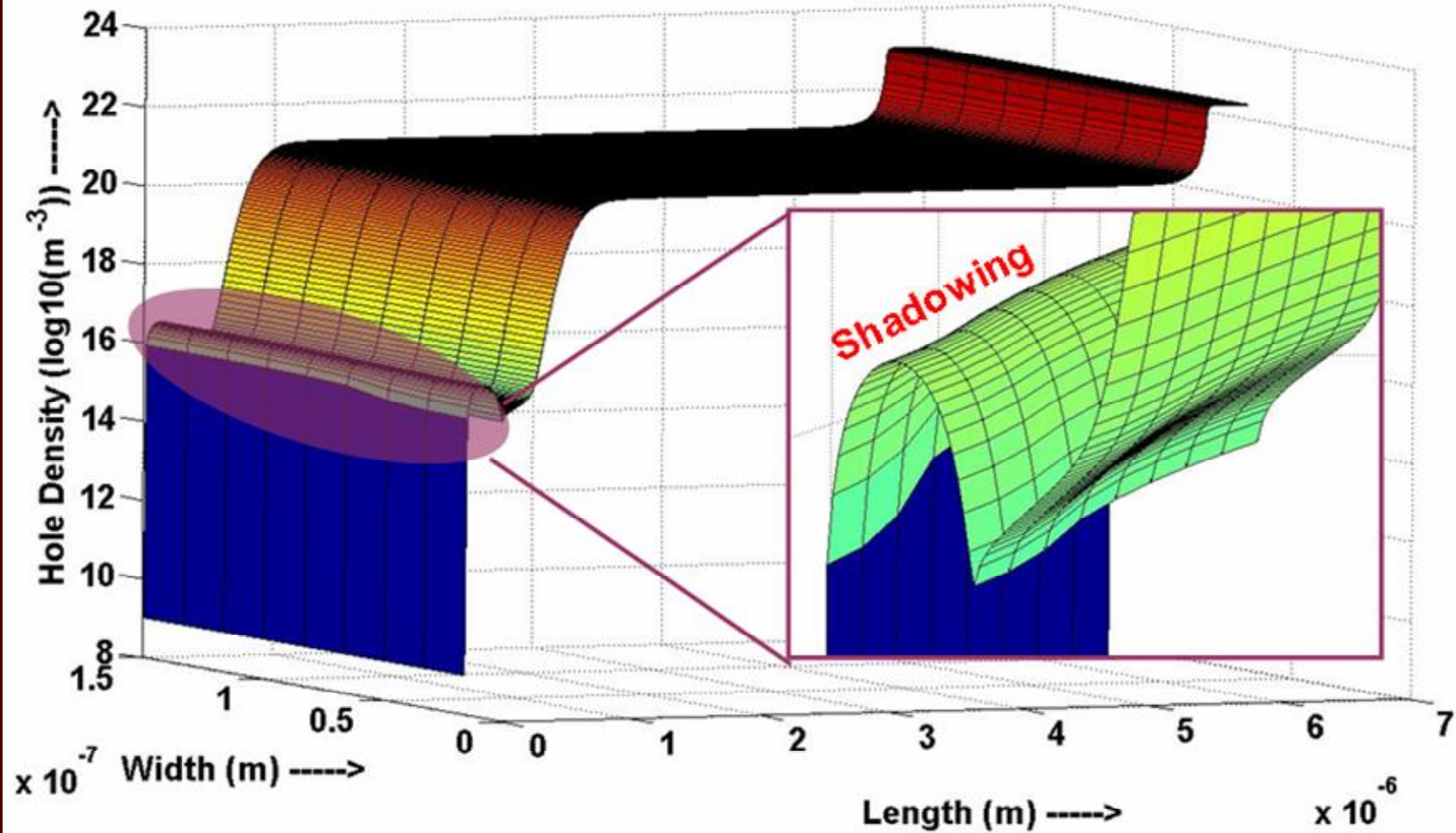


Solar Cell Equations

- Shadowing -

- Light enters through the window normal to the top surface defined by the metal contact.
- No carriers are generated by the light under the metal contact as it is reflected back.
- Carriers generated by light entering through the window diffuse to the region below the metal contact due to density gradient. These carriers generated near the space charge region contribute to the current produced by the solar cell.
- Surface recombination takes place on the surface of the window which reduces the efficiency of the solar cell.

Hole Density Profile Under Illumination



Carrier Density profile in n⁺-p-p⁺ structure displaying shadowing

Solar Cell Equations

- Photon Recycling -

- The re-absorption of photons emitted in a semiconductor material as a consequence of radiative recombinations, a process referred to as photon recycling (PR), has been researched into for several decades because of its primary influence in increasing the minority carrier lifetime and related parameters.
- Solar cells with direct bandgap materials and high-absorption coefficients are firm candidates to show PR effects, leading to an improvement in the conversion efficiency of up to 1-2% in absolute terms for cells with conventional designs.
- However, the formal modeling of PR effects requires the inclusion of additional terms in the standard set of semiconductor equations and researchers usually tend to neglect its influence, because of the lack of available tools for an easy evaluation of this phenomenon in their particular devices.

Solar Cell Equations

- Quantum Efficiency for Current Collection -

- **Quantum efficiency (QE)** is the ratio of the number of charge carriers collected by the **solar cell** to the number of **photons** of a given energy shining on the solar cell. QE therefore relates to the response of a solar cell to the various wavelengths in the spectrum of light shining on the cell. The QE is given as a function of either wavelength or energy. If all the photons of a certain wavelength are absorbed and we collect the resulting minority carriers (for example, electrons in a p-type material), then the QE at that particular wavelength has a value of one. The QE for photons with energy below the **bandgap** is zero
- "Quantum efficiency" is also sometimes called **IPCE**, which stands for **Incident-Photon-to-electron Conversion Efficiency**.

Simulation of Solar Cells With Silvaco

Optical Source Specification

```
# SECTION 5: Optical source specification
#
# define a multi-spectral beam normal to top (y=0.0) surface
# as follows:
# beam #1, origin at (2.5,-1.0), directed at an angle of 90 degrees,
# the beam spectrum is in the file optoex04.spec, the spectrum is
# sampled from 0.5 microns to 0.88 microns with 4 samples.
#
beam    num=1 x.origin=5.0 y.origin=-1.0 angle=90.0 \
        power.file=optoex04.spec wavel.start=0.5 wavel.end=0.8 \
        wavel.num=5
#
```

Obtaining Spectral Response

- The LAMBDA parameter under the SOLVE statement sets the source wavelength.
- Example

```
SOLVE B1=1 LAMBDA=0.2
```

```
SOLVE B1=1 LAMBDA=0.3
```

```
SOLVE B1=1 LAMBDA=0.4
```

```
SOLVE B1=1 LAMBDA=0.5
```

```
SOLVE B1=1 LAMBDA=0.6
```

```
SOLVE B1=1 LAMBDA=0.7
```

```
SOLVE B1=1 LAMBDA=0.8
```

Silvaco Simulations

- Open Circuit Voltage and Short Circuit Current -

- To obtain Voc and Isc first the illumination condition should be defined (multi spectral sources)
- The short-circuit current is obtained by defining the contacts as voltage contacts and obtaining a solution with the device under zero bias with illumination:

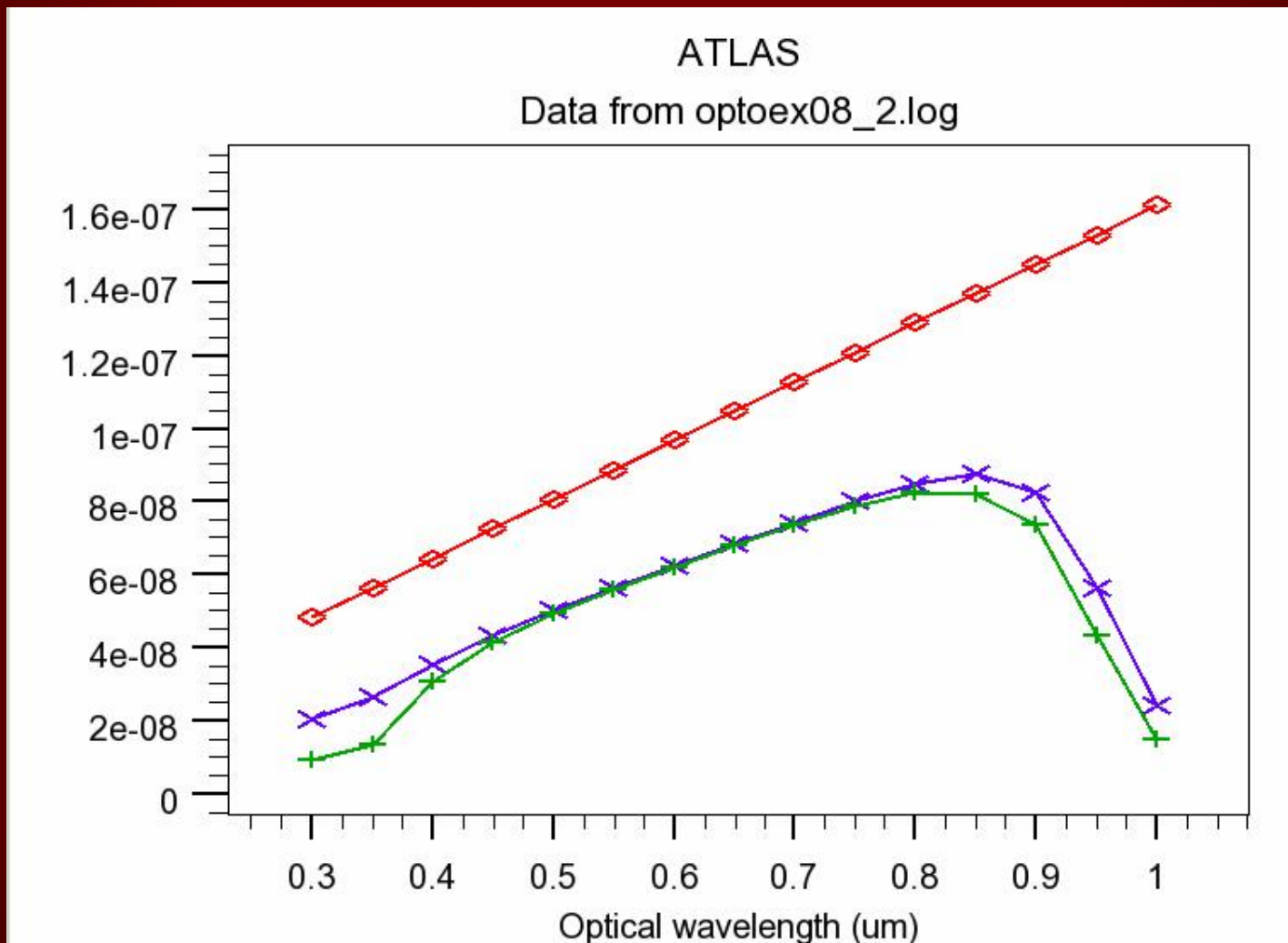
```
SOLVE B1=1.0
```

- The open-circuit voltage is obtained by defining one or more contacts as current controlled and then the current is set to zero:

```
CONTACT NAME=anode CURRENT  
SOLVE I1=0 B1=1.0
```

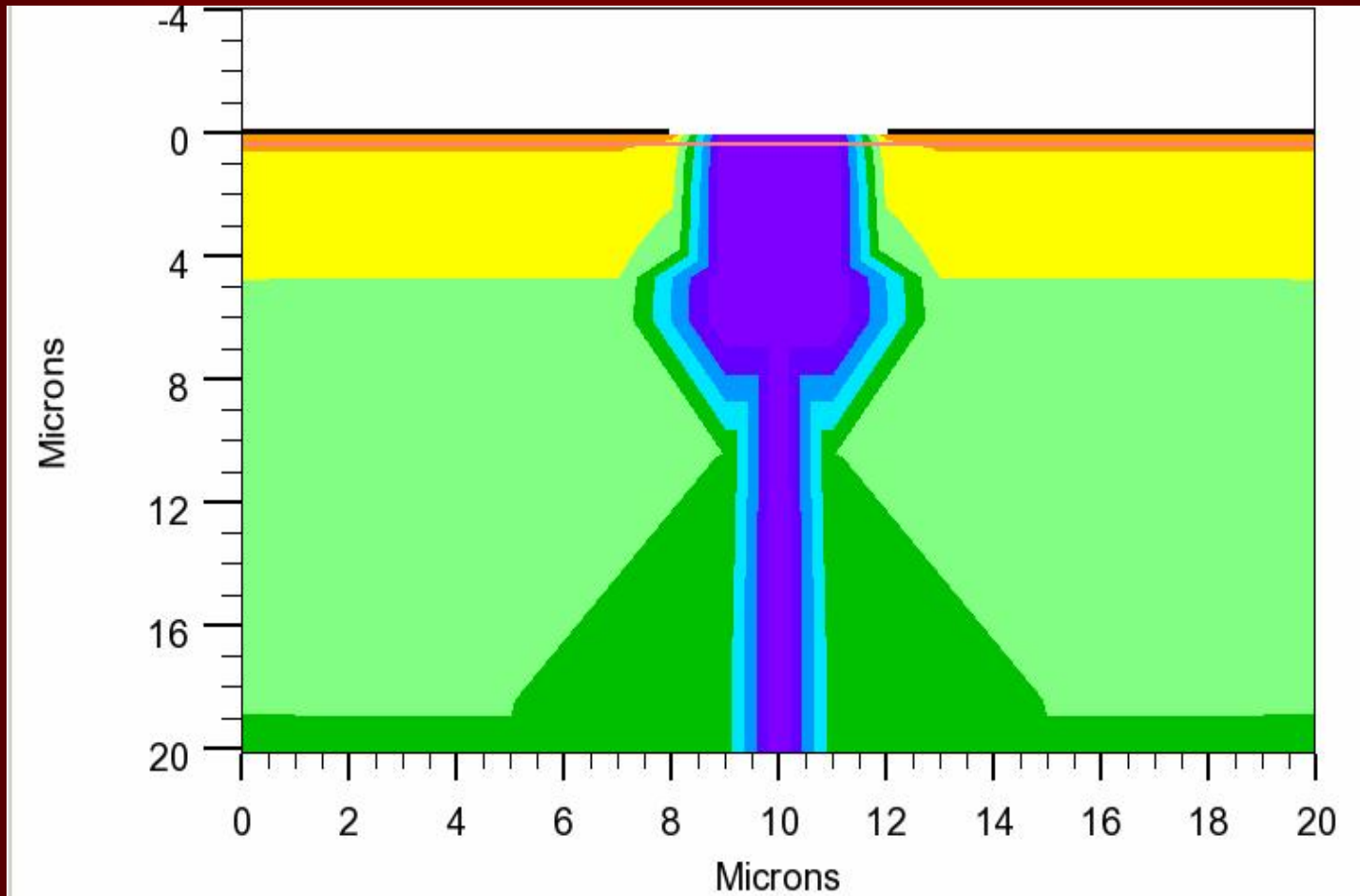

Silvaco Simulations

- Results -



Silvaco Simulations

- Generation Rate -



Silvaco Simulations

- Program Listing -

```
go atlas
```

```
# set contact material to be opaque  
material material=Aluminum imag.index=1000
```

```
material material=Silicon taun0=1e-6 taup0=1e-6
```

```
# set light beam using solar spectrum from external file  
beam num=1 x.origin=10.0 y.origin=-2.0 angle=90.0 power.file=optoex08.spec
```

```
# saves optical intensity to solution files  
output opt.int
```

```
models conmob fldmob srh print
```

```
solve
```