PV Performance Limits by Shockley-Queisser (SQ) Triangle

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Outline

1) Motivation

2) Derivation of the SQ-Triangle

3) Applications of SQ-Triangle

4) Conclusions

5) Appendix: Self-test questions
An Inefficient Machine!

\[ \eta = \eta_N \times \eta_{SQ} \times \eta_M \times \eta_A = \frac{2}{\pi} \times \frac{1}{3} \times \frac{5}{6} \times \frac{1}{2} \sim \frac{1}{10} \]
Power and efficiency

\[ J_{mp} = 82(1 - 0.428E_g) \]

\[ qV_{mp} = 0.95E_g - 0.3 \]
Counting the photons – a roadmap

- **Carnot**
- **Radiative**
- **Below bandgap**
- **Shockley-Queisser**
  - Partition
  - Cell-Module

- **Angle Entropy**

- **Above bandgap**

- **Yablonovitch**

- **LED**
- **CPV**
- **Tandem**
- **MEG**
- **Striping**

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Outline

1) Motivation
2) Derivation of SQ-Triangle
3) Application of SQ-Triangles
4) Conclusions
Defining the SQ-Triangle

1. Calculate $V_{mp}$ and $I_{mp}$

\[ qV_{mp} = 0.95E_g - 0.3 \]
\[ J_{mp} = 82(1 - 0.428E_g) \]

2. Calculate efficiency:

\[ \eta = \frac{V_{mp} I_{mp}}{P_{in}} \]

3. Locate in the triangle

\[ J_{mp} = 72(1 - 0.52V_{mp}) \]
Step 1: Calculate $J_{mp}$

$$J_{mp} = 83.75(1 - 0.428E_g)$$
Step 2: Derive $V_{mp}$ by a 2-Level Atom

Some deep sea Plankton live in a similar diffused light environment.
Detailed balance between Photons and Electrons

Upward transition  \[ = f_2 (1 - f_2) n_{ph} \]

Downward transition  \[ = f_1 (1 - f_2) (n_{ph} + 1) \]

At steady state up and down transitions are equal  \[
\begin{align*}
f_1 (1 - f_2) (n_{ph} + 1) &= f_2 (1 - f_2) n_{ph} 
\end{align*}
\]

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Detailed balance of photons and electrons

\[ f_1 (1 - f_2) (n_{ph} + 1) = f_2 (1 - f_2) n_{ph} \]

\[
\frac{1}{e^{\frac{\theta_1}{T_D}} + 1} \frac{e^{\frac{\theta_2}{T_D}}}{e^{\frac{\theta_1}{T_D}} + 1} (n_{ph} + 1) = \frac{1}{e^{\frac{\theta_2}{T_D}} + 1} \frac{e^{\frac{\theta_1}{T_D}}}{e^{\frac{\theta_1}{T_D}} + 1} \times (n_{ph})
\]

**Bose Einstein distribution**

\[ n_{ph} = \frac{1}{e^{\frac{\hbar \omega}{k_B T_S}} - 1} \]

\[ n_{ph} + 1 = \frac{e^{\frac{\hbar \omega}{k_B T_S}}}{e^{\frac{\hbar \omega}{k_B T_S}} - 1} \]

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PV Efficiency of 2-level System

\[ \frac{E_2 - \mu_2}{T_D} + \frac{E_2 - E_1}{T_S} = \frac{E_1 - \mu_1}{T_D} \]

\[ (\mu_1 - \mu_2) = (E_1 - E_2) \left[ 1 - \frac{T_D}{T_S} \right] \]

\[ \eta = \frac{(\mu_1 - \mu_2) R}{(E_1 - E_2) R} = \left[ 1 - \frac{T_D}{T_S} \right] \]

\[ \eta = \left[ 1 - \frac{300}{6000} \right] = 0.95 \]

Single molecule-single frequency gives Carnot efficiency!

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Problem of Angular Anisotropy

\[ \theta_2 f_1 (1 - f_2)(n_{ph} + 1) = \theta_1 f_2 (1 - f_2)n_{ph} \]

or, \[ -\ln\left(\frac{\theta_1}{\theta_2}\right) + \left(\frac{E_2 - \mu_2}{k_B T_D}\right) + \left(\frac{E_1 - E_2}{k_B T_S}\right) = \left(\frac{E_1 - \mu_1}{k_B T_D}\right) \]

\[ \therefore \mu_1 - \mu_2 = V_{mp} = E_g \left(1 - \frac{T_D}{T_S}\right) + k_B T_D \ln\left(\frac{\theta_1}{\theta_2}\right) \quad \text{negative number} \]

The angle mismatch leads to Vmp loss
Step 1: Derivation of $V_{mp}$ complete

\[ \theta_1 = 6 \times 10^{-5} \]

\[ \theta_2 = 4\pi \quad \text{Without mirror} \]

\[ \theta_2 = 2\pi \quad \text{With mirror} \]

\[ \eta = \frac{\mu_1 - \mu_2}{E_1 - E_2} = \left(1 - \frac{T_D}{T_S}\right) + \frac{k_BT_D}{E_1 - E_2} \ln\left(\frac{\theta_1}{\theta_2}\right) \]

Set $T_S = 6000 K, T_D = 300 K,$

\[ E_g = E_1 - E_2, \theta_2 = 2\pi : \]

\[ qV = \Delta \mu = \left(1 - \frac{T_D}{T_S}\right)E_g + k_BT_D \ln\left(\frac{\theta_1}{\theta_2}\right) = 0.95 \times E_g - 0.31 \]

Consistent with all experimental data!
Concentrator cells fool the cells

\[ \theta_{S,C} = \theta_D \]

Number of suns \( N = \frac{2\pi}{\theta_S} \approx 104720 \)

\[ V_{mp} = \left(1 - \frac{T_D}{T_S}\right)E_g + k_B T_D \ln \left(\frac{\theta_S}{\theta_D}\right) \rightarrow \left(1 - \frac{T_D}{T_S}\right)E_g \]

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Step 3: Creating the SQ Triangle

\[ qV_{mp} = E_g \left(1 - \frac{T_D}{T_S}\right) - k_B T_D \ln \left(\frac{\theta_D}{\theta_S}\right) \]

\[ = c_f E_g - \Delta \]

\[ J_{mp}(E_g) = cI_{sun}(1 - \beta' E_g) \]

\[ = J_0 \left(1 - \beta V_{mp}\right) \]

\[ \beta \equiv \beta' / c_f \]

\[ V_0 \equiv \frac{(1 - \beta \Delta)}{\beta} \]

\[ J_0 \equiv cI_{sun} \left(1 - \beta \Delta\right) \]

Hirst, PIP, 2011
Khan & Alam, APL, 2015,
Also, see AJP, 2012
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4) Conclusions
Maximum Single Junction Efficiency

\[ S_1 = x(1-x) \]
\[ \frac{dS_1}{dx} = 1 - 2x = 0 \rightarrow x = \frac{1}{2} \]

\[ J_{mp} = 72(1 - 0.52 V_{mp}) \]

\[ 0.52 \times V_{mp} = \frac{1}{2}, \quad V_{mp} = 0.96, \quad 0.95 \times E_g - 0.3 = V_{mp} = 0.96, \quad E_g = 1.33V \]

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Tandem Solar Cell

\[ E_0 \leq E_{i+} \leq E_{1+} \leq E_Q \]

(b)
N-Junction Tandem Cell

\[ V_{mp} = c_f E_g - 0.31 - k_B T_D \ln c \]

\[ E_{g,1}, V_{mp,1} \]
\[ E_{g,2}, V_{mp,2} \]
\[ E_{g,3}, V_{mp,3} \]

\[ V_{mp} = iV_0/(N + 1) \]
\[ I_{mp}^{(i)} = I_0/(N + 1) \]

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Efficiency of N-junction Tandem

\[ \eta_N (c) = \left( \frac{I_0 \cdot V_0}{4c} \right) \times \frac{2N}{N+1} \]

Equations:

\[ V_0 \equiv \frac{(1 - \beta \Delta)}{\beta} \]
\[ I_0 \equiv cI_{sun} (1 - \beta \Delta) \]
\[ \beta = \frac{\beta'}{c_f} \]

Graphs are shown to illustrate the efficiency and mathematical expressions for tandem solar cells.
Tandem Efficiency Limits

\[ J_{mp} = 70(1 - 0.52 \, V_{mp}) \]

\[ P_{out} = J_{mp} \times V_{mp} \]

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Bifacial Solar Cell

\[ \eta = \eta_N \times \eta_{SQ} \times \eta_M \times \eta_A = \frac{2}{\pi} \times \frac{1}{3} \times \frac{5}{6} \times \frac{1}{2} \sim \frac{1}{10} \]

\[ \eta_A \sim 1/2 \]
For inverted bifacial design

\[ J_{mp} / J_0 = 1 \]

\[ V_{mp} / V_{01} = 1 \]

\[ (1 - 2x - x) \gamma = 1 / (1 + R) \]

\[ S_4 = x(1 - x) + x (1 - 2x) + x (1 - 2x - x) + x \left(1 - \frac{x}{R}\right) \]

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SQ Triangle for Bifacial PV

\[ S_N = \frac{2(1 + R)N^2}{N(N + 1)(R + 1) - 2R} \]

\[ S_{N} \quad \frac{1}{S_1} = \frac{8R(1 + R)N^2}{2R(2N^2 + 4N - 1) - R^2 - 1} \]

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Advantages of Bifacial PV

\[ N_{\text{crit}} \leq 1 + R^{-1} \]

\[
\frac{S_N}{S_1} = \frac{2(1 + R)N^2}{N(N + 1)(R + 1) - 2R} \\
\frac{S_N}{S_1} = \frac{8R(1 + R)N^2}{2R(2N^2 + 4N - 1) - R^2 - 1}
\]
Plant-PV Tandem cells

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Rescaled Tandem System

For plants

$J_{SC}(X_g) = J_{SUN}(1 - \beta X_g)$

With the new parameters we can now redesign any N-J tandem

$J_{SUN} \quad 83.75 \text{ mA/cm}^2$
$\beta \quad 0.428 \text{ eV}^{-1}$

$J_{SUN}^\text{new} \quad 63.2095 \text{ mA/cm}^2$
$\beta^\text{new} \quad 0.5666 \text{ eV}^{-1}$

$J_{SC}^\text{new}(X_g) = J_{SUN}(1 - \beta X_g) - J^\text{cut}
= J_{SUN}(1 - \beta^\text{new} X_g)$

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Conclusions

• Solar cells are inefficient machines. A thermodynamic analysis shows how we can improve the performance.

• A simple SQ Triangle anticipates thermodynamic limits for tandem PV, bifacial PV, and concentrator PV cells.

• Tandem efficiency scales as: \( \eta_N(c) = I_0 V_0 N/[2(N + 1)c] \)

• Bifacial PV has phase transition at \( N_{crit} \leq 1 + R^{-1} \)

• Thermodynamic limit serves as a beacon and a guardrail for next generation PV.

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Single (SJ) or multi-junction (MJ)
SJ: J-V or Eg-sweep
MJ: J-V or N-sweep
Input spectrum: AM1.5G or ideal Blackbody
Distance from sun (for Blackbody input)
Spectral low-pass filter (for MJ calculations)
Reflectance of the ground (for MJ calc.)

Simulation setup
- Single (SJ) or multi-junction (MJ)
  - SJ: J-V or Eg-sweep
  - MJ: J-V or N-sweep

Simulation specific input
These set of inputs change based on the choice of simulation setup

Spectral input
- Input spectrum: AM1.5G or ideal Blackbody
- Distance from sun (for Blackbody input)
- Spectral low-pass filter (for MJ calculations)
- Reflectance of the ground (for MJ calc.)

nanohub.org/resources/pvlimits
http://arxiv.org/abs/1606.01176
Self-assessment

1. How does the average bandgap of tandem cell compare to that of a single junction solar cell?

2. How does the efficiency of a triple junction solar cell compare to that of a single junction solar cell? Hint. Efficiency ratio is given by $\frac{2N}{N+1}$.

3. What is the maximum short-circuit current achievable from AM1.5 illumination? Ans. 70 mA/cm$^2$.

4. What is the maximum short circuit current for a 4-junction solar cell? Ans. $\frac{70}{N+1} = 14$ mA/cm$^2$

5. For $R=0.3$, what is efficiency of a 4-junction bifacial solar cell?

6. If $R_s$ increases by a factor of 5, how much does the critical concentration for a CPV decrease by?
Maximum J_{sc} (in mA/cm^2) from AM1.5 spectrum is

a) 7000    b) 700    c) 70    d) 7

70 mA/cm^2
Wait, Wait don’t tell me …

Maximum Jsc for Eg=1.7 eV perovskite under AM1.5 illumination is

a) 100  b) 50  c) 20  d) 5

Jsc=83.75(1-0.43Eg) =23 mA/cm²
Wait, Wait don’t tell me …

For a 3-junction tandem, maximum $J_{sc}$ in mA/cm² is

a) 100  b) 70  c) 17  d) 4

$$J_{sc} = \frac{J_{max}}{(N+1)}$$
Wait, Wait don’t tell me …

If $E_g = 1 \text{eV}$, maximum $V_{mp}$ is

a) 1.0  b) 0.65  c) 0.45  d) 0.25

$V_{oc} = 0.95E_g - 0.31$
In a N=3 tandem, $E_1=1.9\text{eV}$, $E_3=0.97$, what is $E_2$?

a) 2.5  

b) 1.6  

c) 1.3  

d) 1.1

\[ E_{g,\text{ave}} = E_{g,SJ} = 1.33 \]
Wait, Wait don’t tell me …

In a $N=3$ tandem, What is $V_{mp}$?

a) 4  b) 3  c) 2  d) 1

$V_{mp}/N=0.95E_{avg}-0.3I$
A Little Formula Sheet

**SJ cell**

\[ J_{sc,SJ} = J_0 \left( 1 - \beta E_g \right) \quad \text{(AM1.5, } J_0 = 83.75, \beta = 0.428 \text{).} \]

\[ qV_{oc,SJ} = 0.95 \times E_g - 0.232 \]

\[ qV_{mp,SJ} = 0.95 \times E_g - 0.31 \]

\[ E_{g,SJ}^{opt} \approx 2.55 \ kT_s \]

\[ FF \sim (v_{oc}/v_{oc} + 4.7) \]

\[ \eta_{T,SJ} = -26.45E_g^2 + 70.77E_g - 14.42 \quad \text{(AM1.5, empirical)} \]

**Tandem**

\[ J_{sc}(N) = \frac{2}{N+1} J_{sc}(\langle E_g \rangle) \]

\[ qV_{mp}/N = \langle E_g \rangle \left( 1 - \frac{T_D E_{g,max}}{\langle E_g \rangle T_s} \right) - k_B T_D \ln \frac{\theta_D}{\theta_S} \]

\[ E_{g,max} = \frac{N - 1}{\beta N} + \frac{\beta (1 + R) E_0 - R}{\beta \times N} \]

**Module**

\[ (T - T_a) = P/h = 1000(1 - \eta - R)/h \]

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