

# CIGS Solar Cell Optimization



Using Silvaco's TCAD to Gain a Competitive Advantage



**SILVACO**



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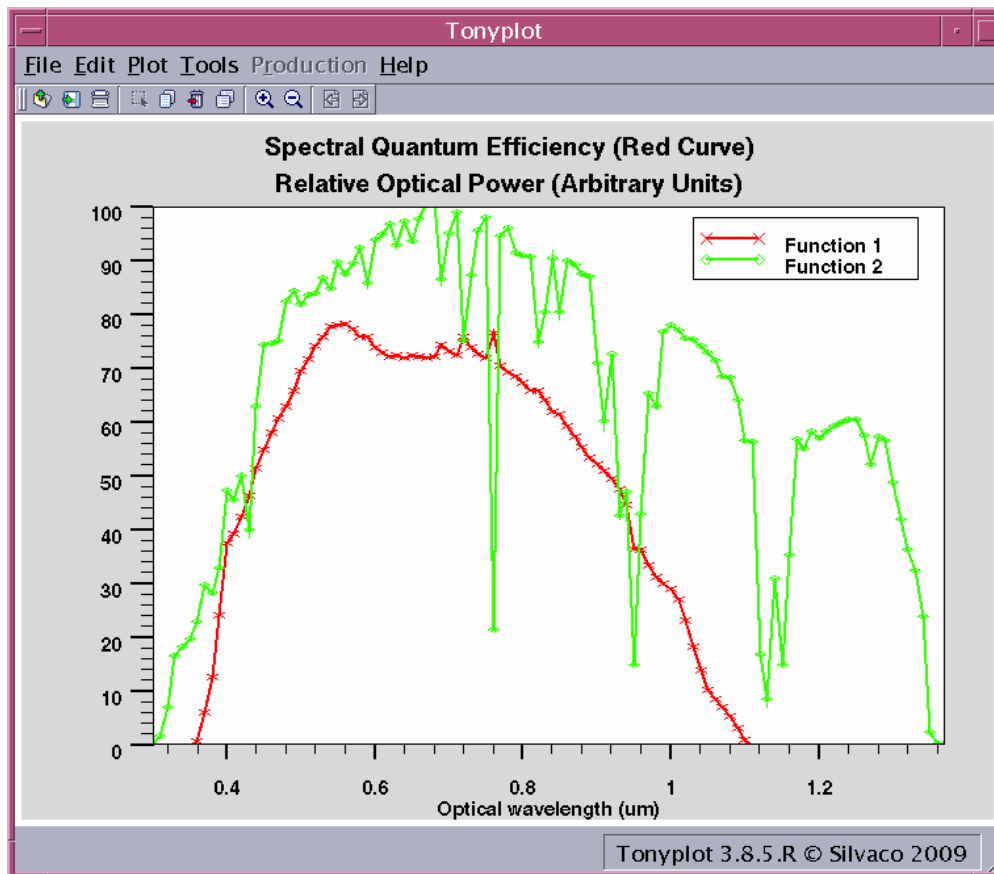
## Introduction

- A standard CIGS / CdS solar cell was constructed using Silvaco's ATLAS/Blaze device simulator
- Spectral response, photo-generation rate versus depth and power output of a complete panel were simulated
- The solar cell was then optimized using ZnO oxide thickness, CdS thickness, Effective Doping and CIGS composition as variables
- For each variable simulated, a response surface model was also constructed using the VWF environment and the results of this response surface model were compared to the simulations
- Finally a brief description of how VWF was used to create the complete R.S.M. is provided at the end



## Baseline Device

- Quantum Efficiency Spectral Response (Red Curve)



The green curve shows the relative spectral response of the “Source Photo Current.”

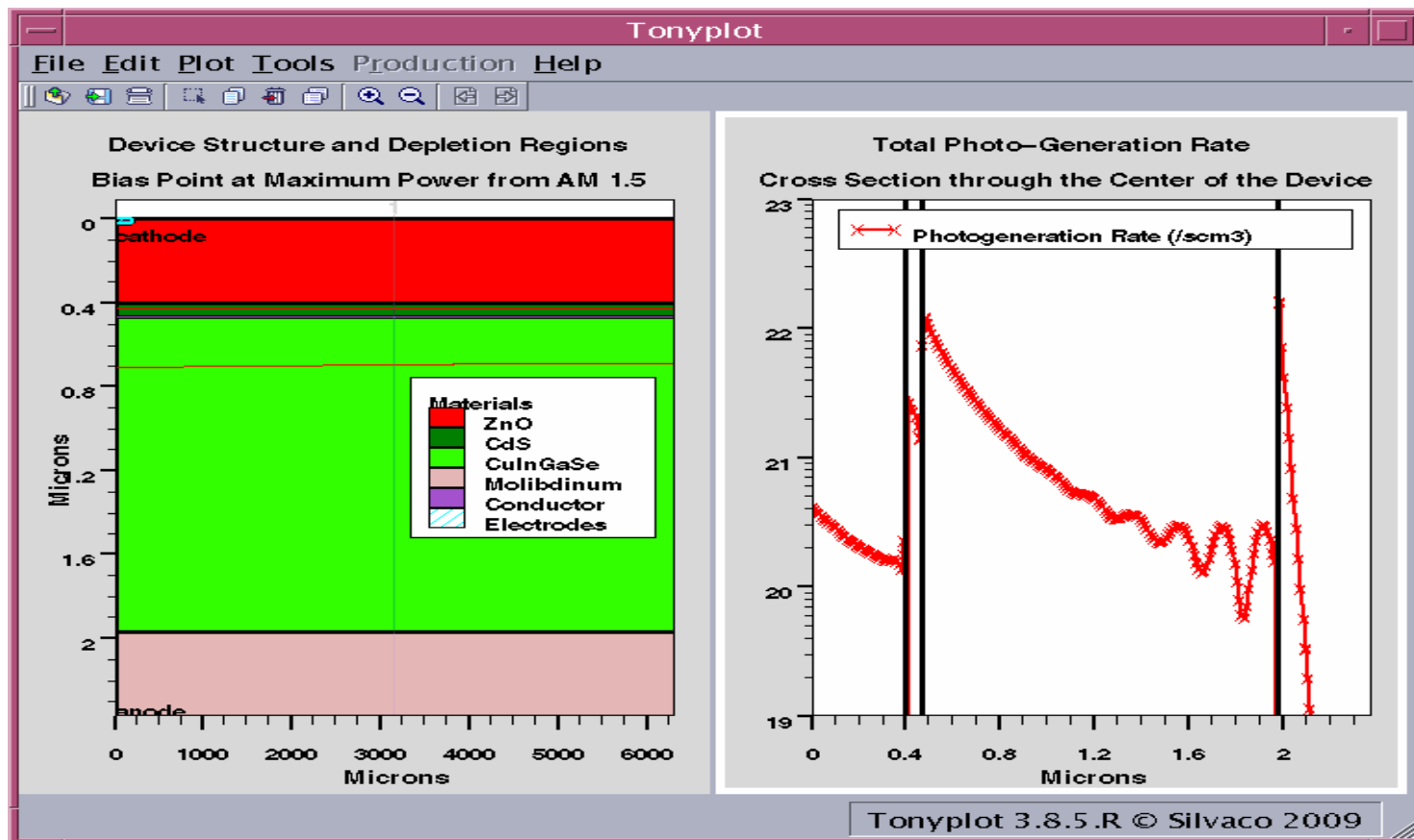
Significant untapped power in the infra-red spectrum.

Q.E. defined here as  
“(Output Current) /  
(Source Photo Current)”  
x100%.



# Baseline Device

- Total Photo-Generation Rate through the device center





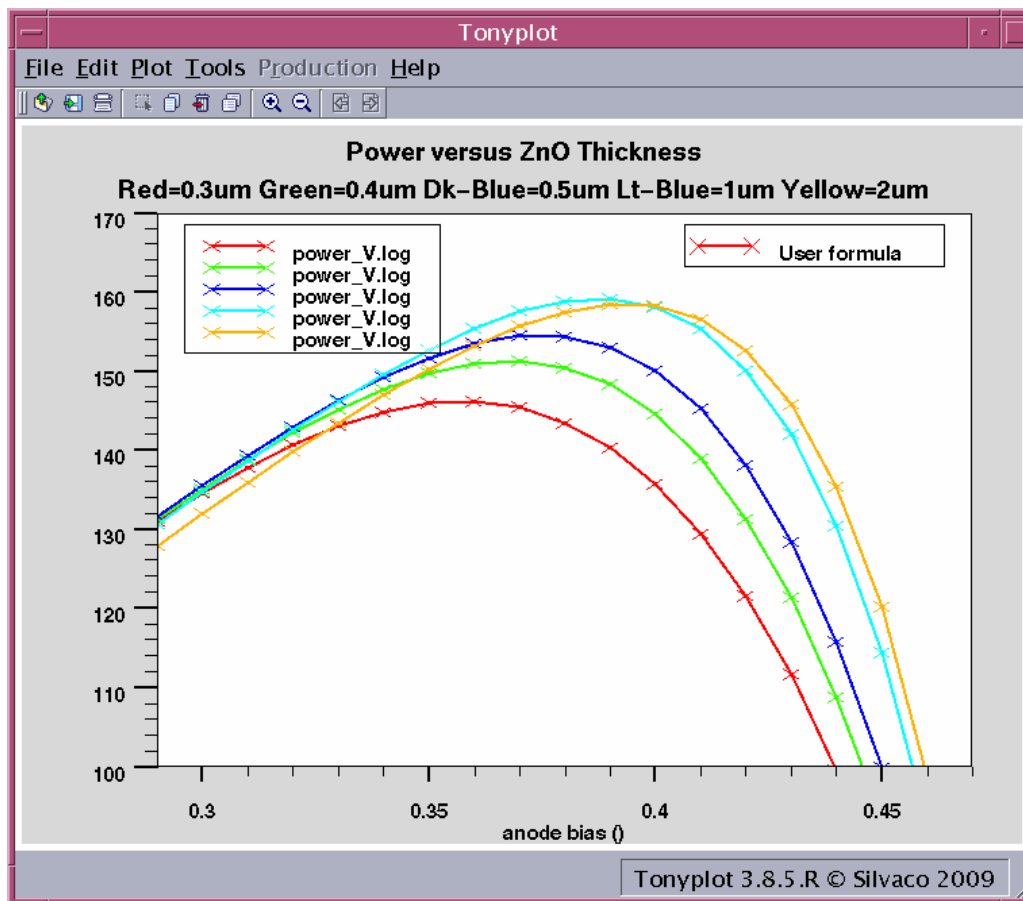
## Baseline Device

- The variance of the depletion width across the device suggests that there is a significant series resistance effect originating from the resistivity of the ZnO contact
- However, the ZnO contact absorbs some of the available light energy i.e., it is not totally transparent
- If the ZnO contact is made thicker to reduce series resistance, it will become more opaque. Clearly there is a trade-off between reducing resistive loss and reducing light loss due to absorption in the “transparent” ZnO contact.
- The first Design of Experiments aims to optimize the ZnO contact thickness.



# Zinc Oxide Conductor Thickness Effects

- Effect of ZnO thickness on Maximum Power Output



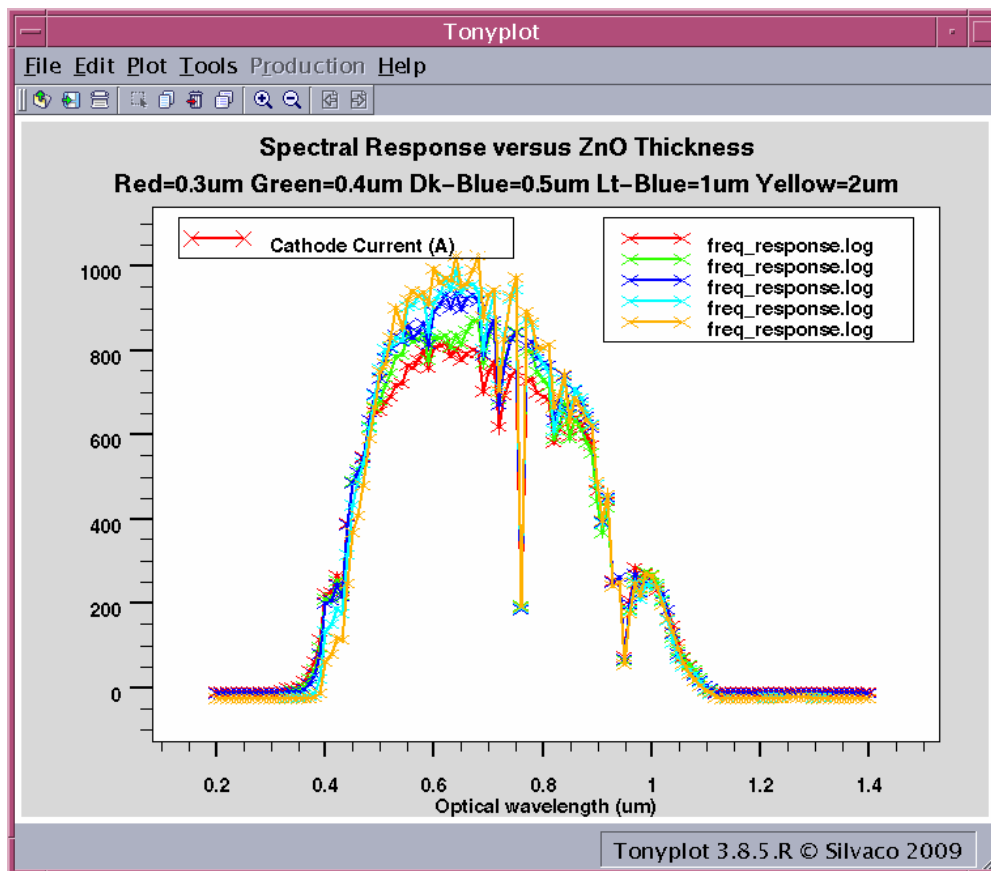
Power – Voltage curves for ZnO thicknesses of 0.3um, 0.4um, 0.5um, 1um and 2um.

Optimum thickness is approximately 1um.



# ZnO Conductor Thickness Effects

- Effect of ZnO Thickness on Spectral Response



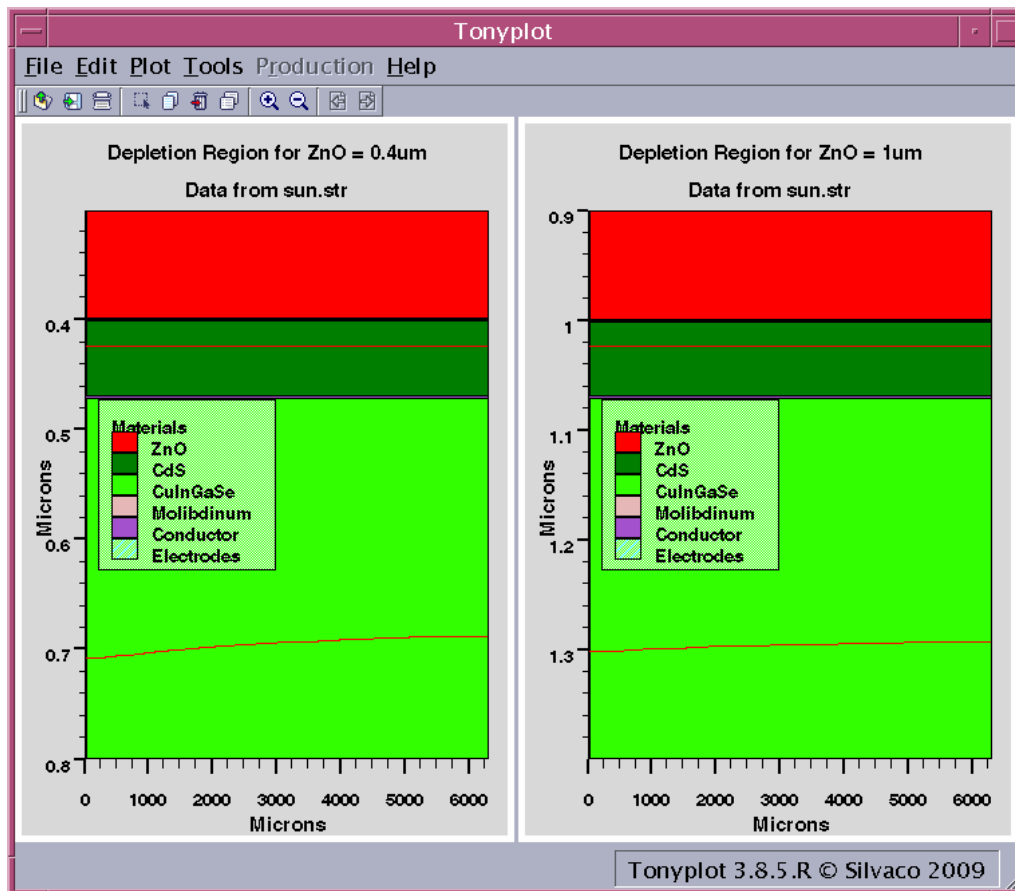
Relative Spectral Contribution to Output Current for ZnO = 0.3um, 0.4um, 0.5um, 1um and 2um.

Device Current increases with ZnO thickness for all but the shortest wavelengths.



# ZnO Conductor Thickness Effects

- Effect of ZnO Thickness on Depletion Width



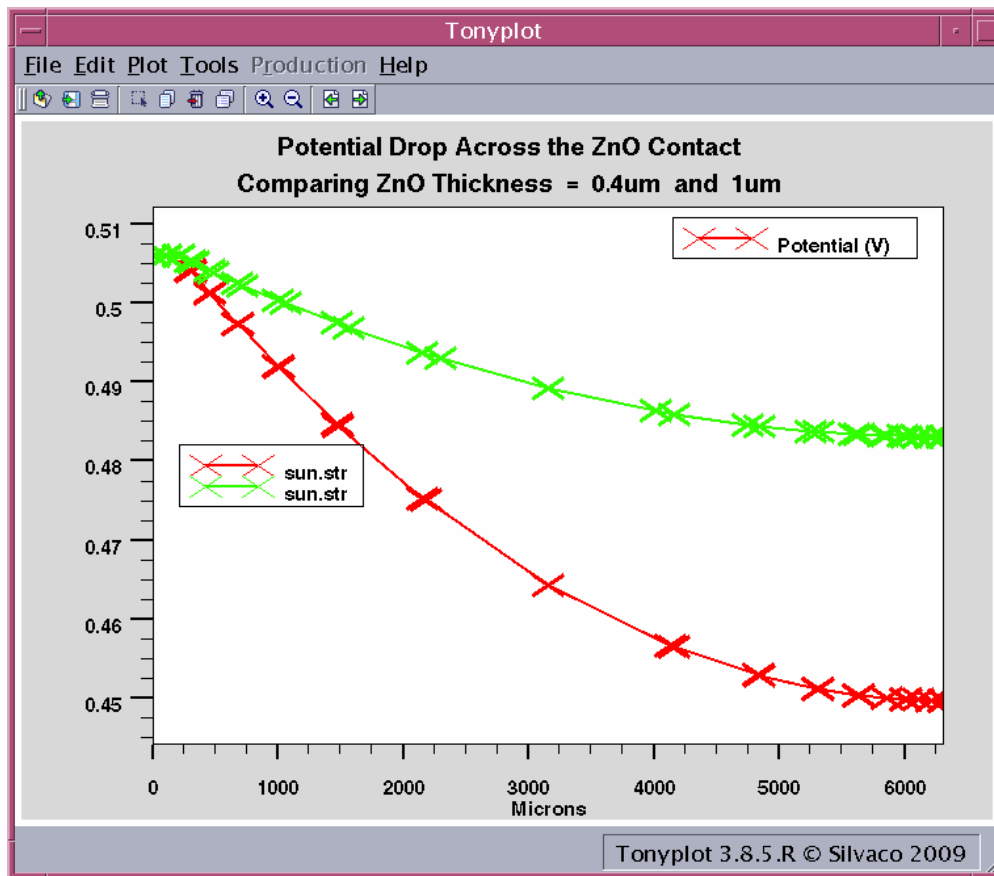
Depletion Width Variation across the device for ZnO thicknesses of 0.4um and 1um.

A thicker ZnO conductor reduces the Voltage Drop across the device



# ZnO Conductor Thickness Effects

- Effect of ZnO Thickness on Contact Potential Drop



Potential Drop across the ZnO Surface Contact for ZnO thicknesses of 0.4um (Red Curve) and 1um (Green Curve).

This potential drop reduces Output Power and Efficiency.



## ZnO Conductor Thickness Effects

```
Text Editor V3.8 - performance.txt
File View Edit Find
Effect of Increasing ZnO thickness
----->
ZnO Thickness = 0.4um (Baseline Device Value)
-----
Short Circuit Panel Current = 2.49328 Amps
Open Circuit Panel Voltage = 92.7348 Volts
Panel Current at Maximum Power = 2.15215 Amps
Panel Voltage at Maximum Power = 70.3 volts
Max Power (Watts/panel) = 151.296
Conversion Efficiency = 0.0769719
ZnO Thickness = 1um
-----
Short Circuit Panel Current = 2.46234 Amps
Open Circuit Panel Voltage = 92.6256 Volts
Panel Current at Maximum Power = 2.14848 Amps
Panel Voltage at Maximum Power = 74.1 volts
Max Power (Watts/panel) = 159.203
Conversion Efficiency = 0.0809946
```

These are the numbers you are really interested in.

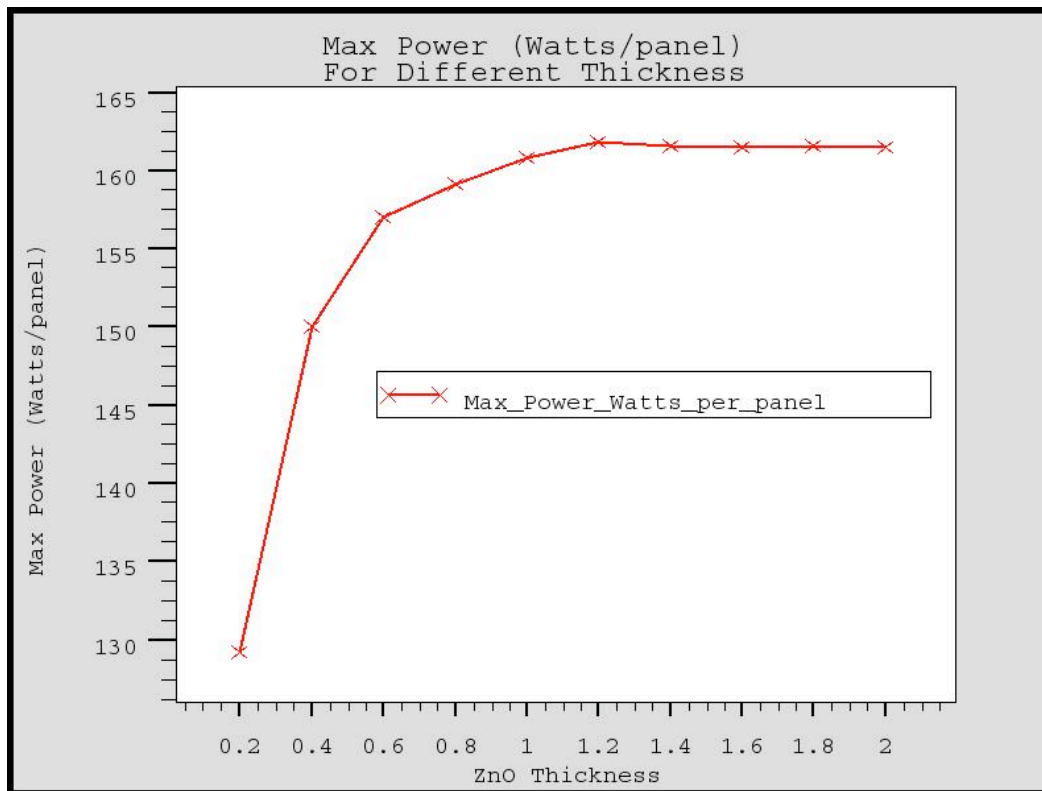
Max Power increased from 151 W to 159 W.

Max Efficiency increased from 7.7% to 8.1%.



# ZnO Conductor Thickness Effects

- Output from running VWF Experiments



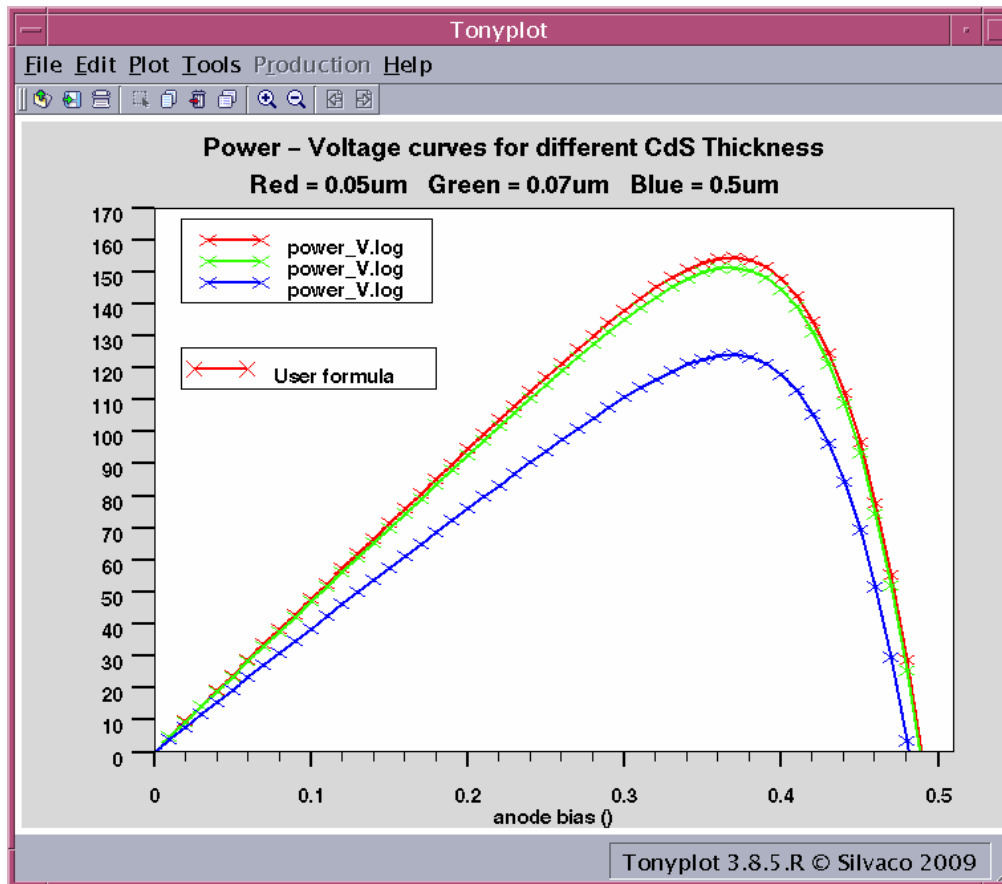
Maximum Output Power versus ZnO Thickness.

Significant gains for ZnO thickness around 1.15um thick.



## CdS Thickness Effects

- Effect of CdS Thickness on Maximum Power Output



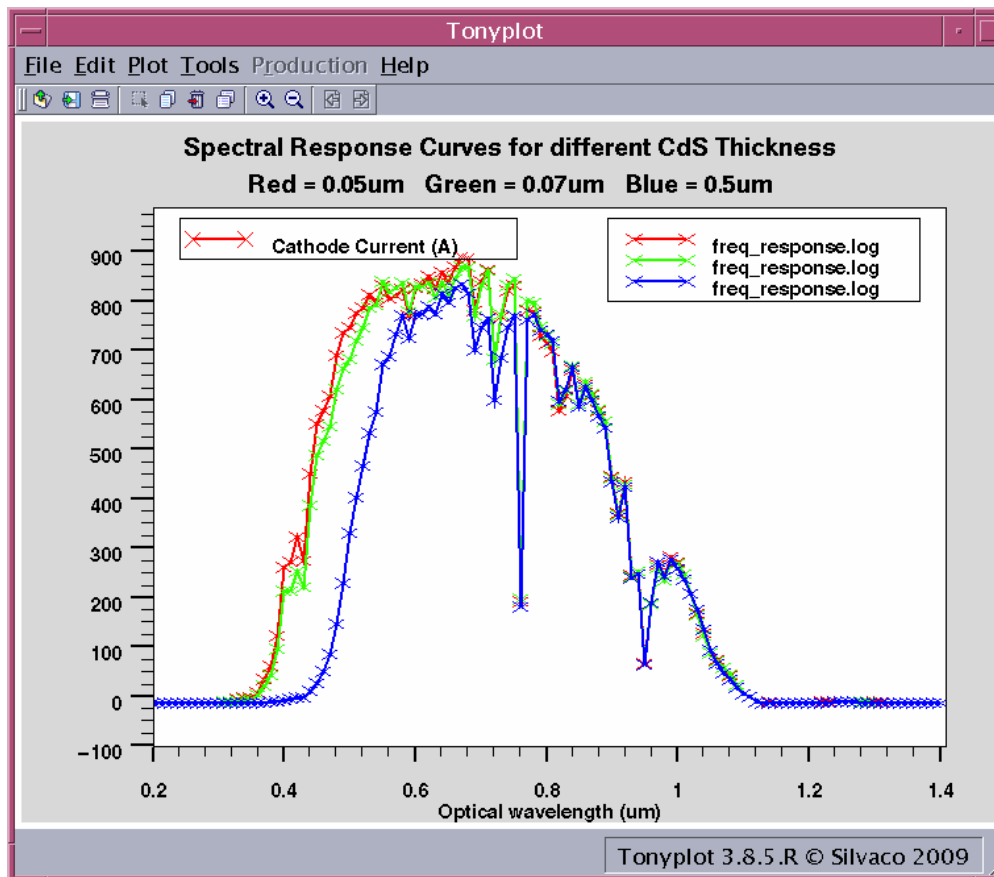
Simulated thickness of 0.05um (Blue), 0.07um (Green) and 0.5um (Red).

No benefit gained from increasing CdS thickness.



# CdS Thickness Effects

- Relative Spectral Contribution to Output Current

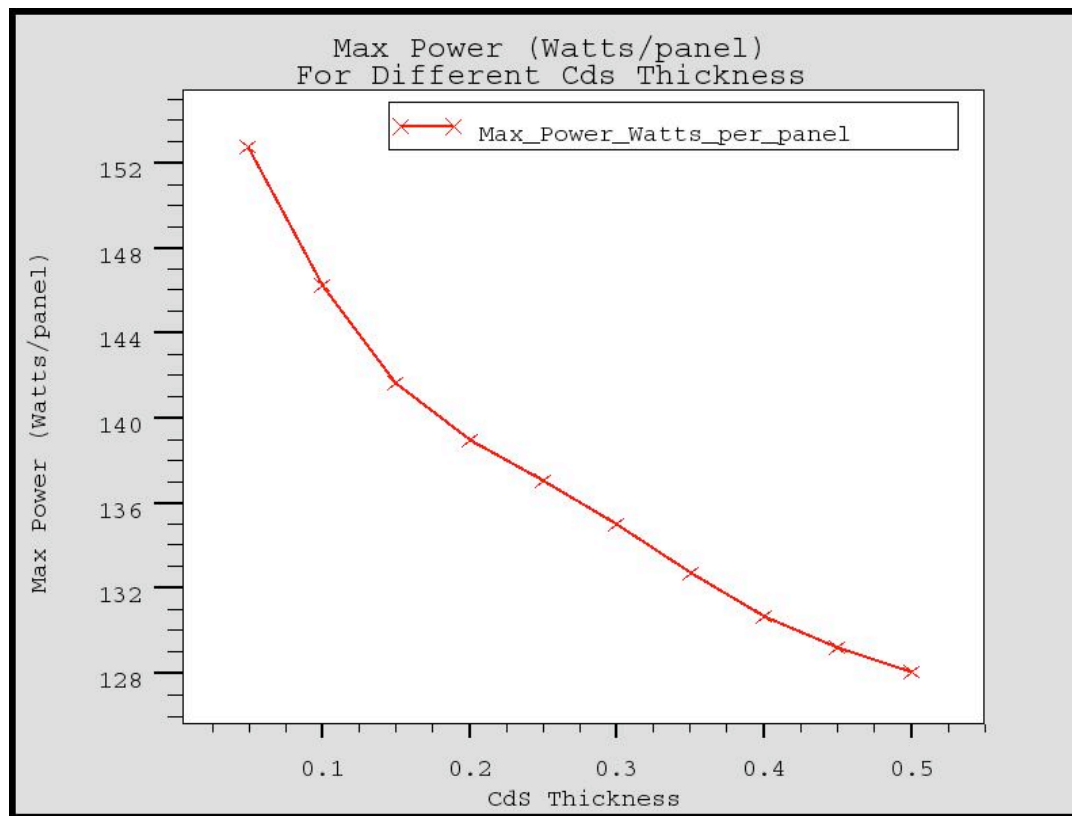


Thicker CdS layer absorbs wavelengths shorter than 0.5um as expected but these generated carriers do not contribute to output current.



## CdS Thickness Effects

- Output from running VWF Experiments



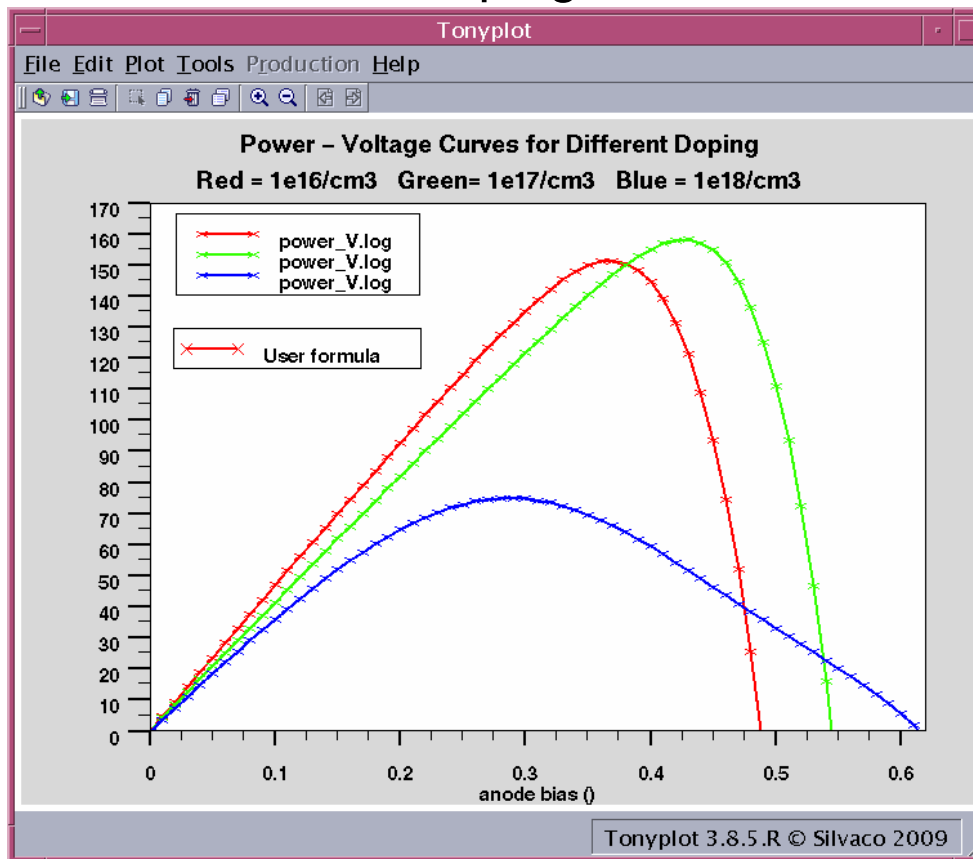
Maximum Output Power (Y axis) versus CdS n-type layer Thickness (X-axis).

This layer needs to be kept as thin as possible so long as it is not fully depleted.



# CIGS Effective Doping Concentration Effects

## ■ Effect of CIGS Doping on Power – Voltage Curve

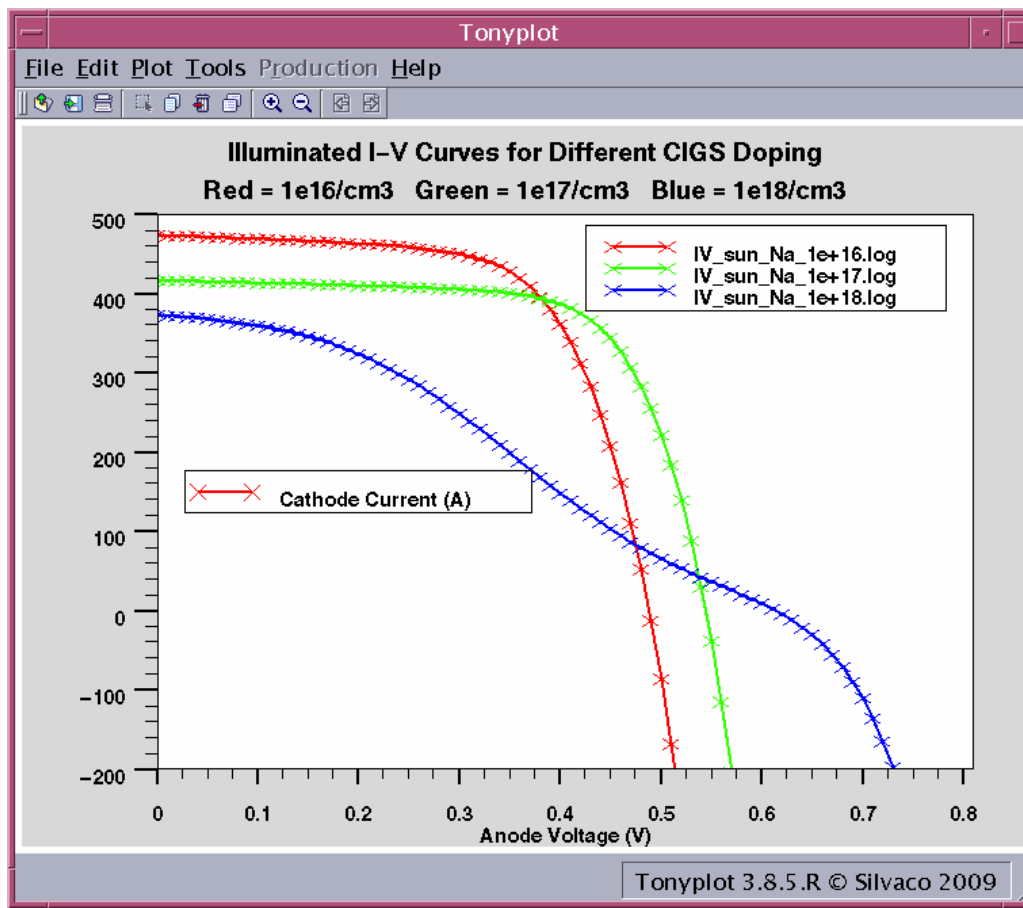


There is a maximum power advantage if CIGS Effective Doping could be increased to around  $1e17/cm^3$ .



# CIGS Effective Doping Concentration Effects

## ■ I-V Curves versus Effective Doping

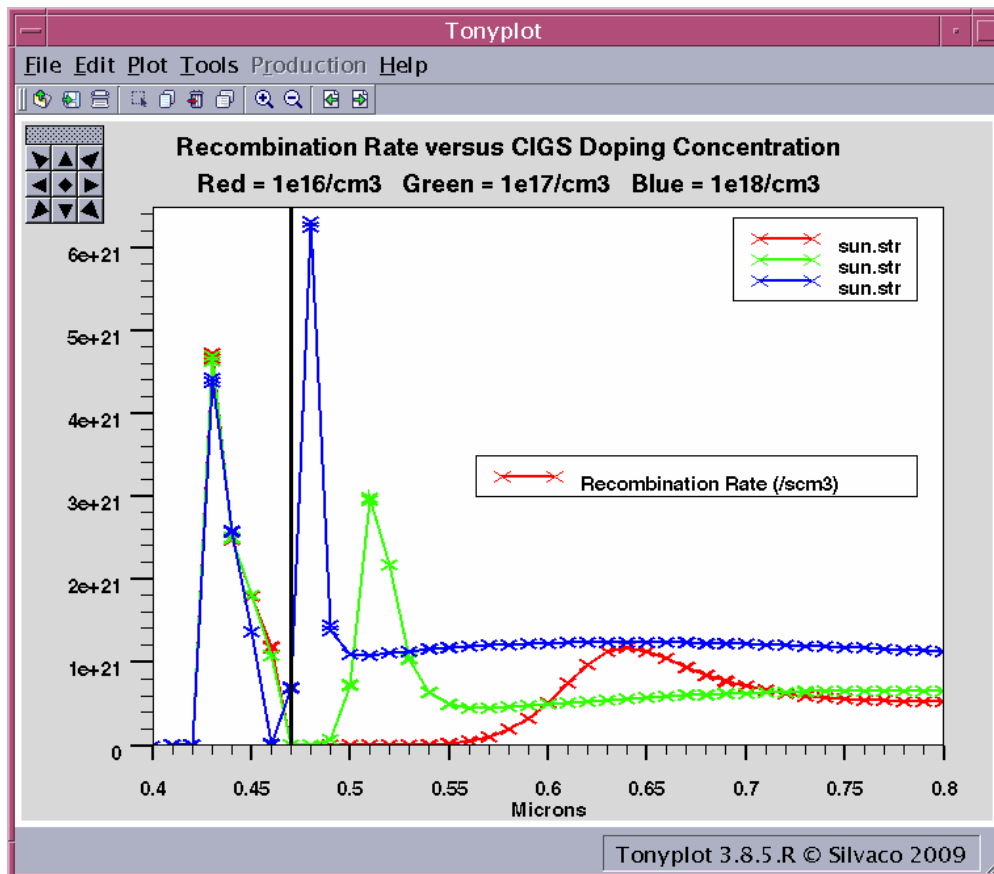


The Increased Power results from the Increased Output Voltage more than make up for reduced output current from reduced efficiency at longer wavelengths.



# CIGS Effective Doping Concentration Effects

- Recombination Rate versus Effective CIGS Doping

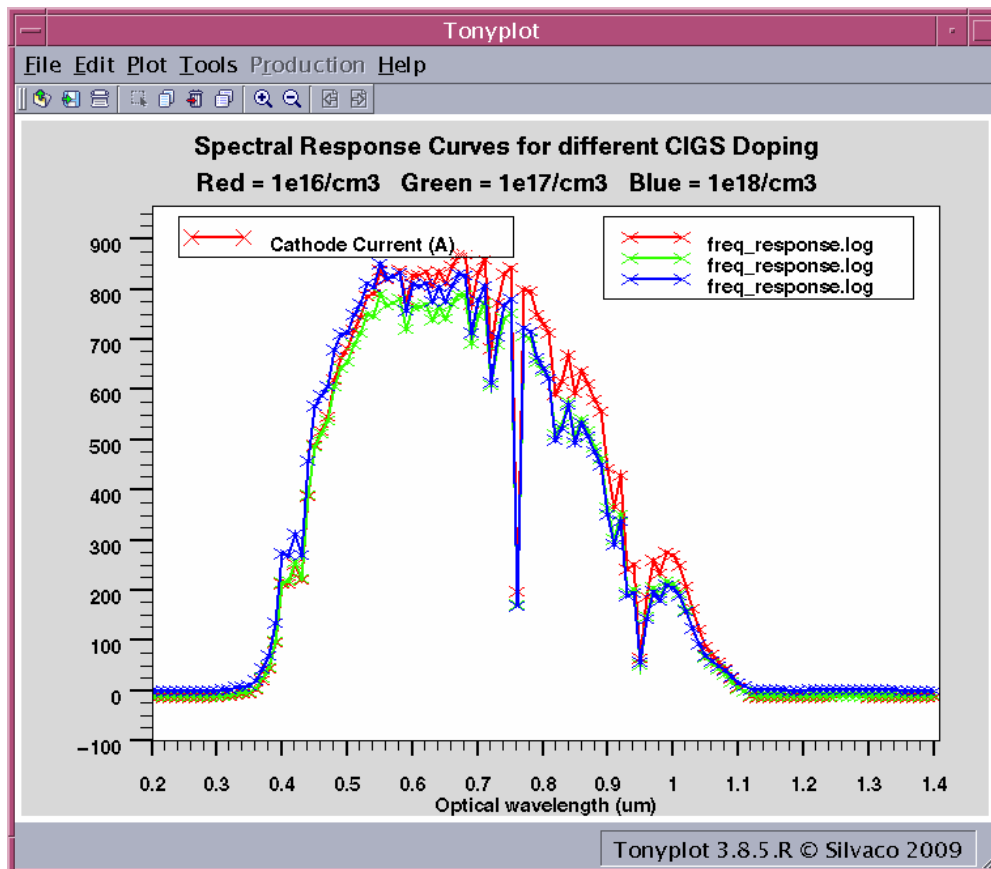


Increased Recombination for higher doping levels greatly reduces electron hole pair separation yield.



# CIGS Effective Doping Concentration Effects

- Spectral Response of Current versus CIGS Doping



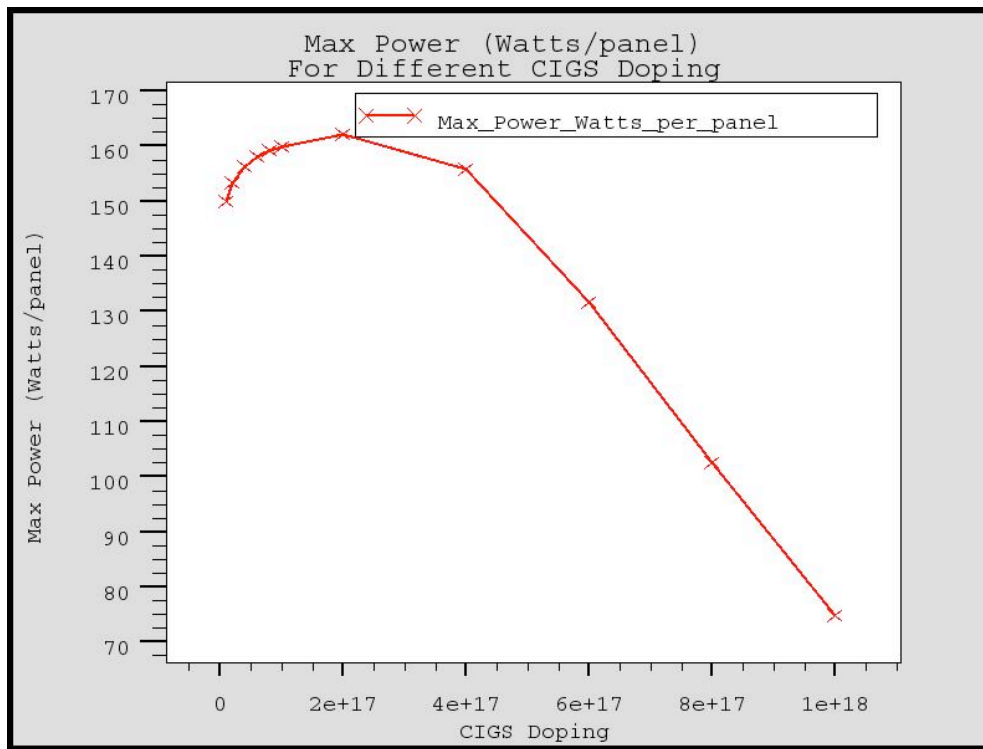
Higher Doping Increases Yield at Shorter Wavelengths but Reduces Yield at Longer Wavelengths.

This is similar to Increasing the Band-Gap of the CIGS Film, so this is the next experiment to try.



## CIGS Effective Doping Concentration Effects

- Output from running VWF Experiments



Maximum Power versus CIGS Doping.

Maximum Power Output at approximately  $2e17/cm^3$ .

This suggests increasing the CIGS bandgap could be beneficial.



## CIGS X-Composition (Band-Gap) Effects

- Cu In(1-X) Ga(X) Se<sub>2</sub> Band-Gap versus X-Composition

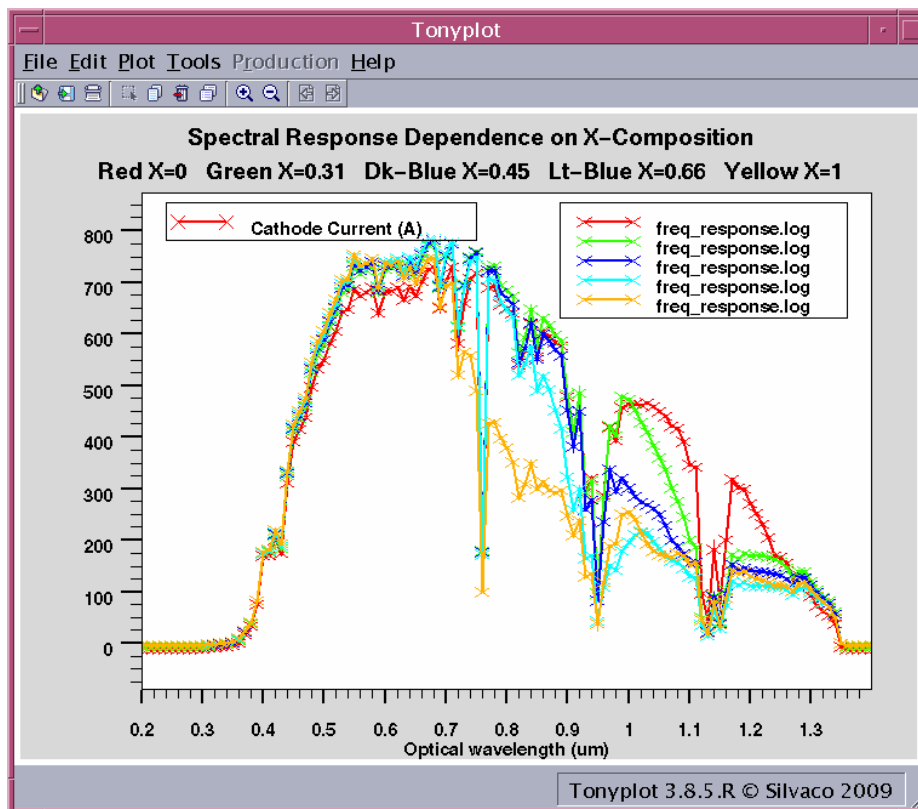
X-Comp.	Band-Gap	Lambda
0	1.0696 eV	1.159 um
0.31	1.2798 eV	0.969 um
0.45	1.3760 eV	0.901 um
0.66	1.5218 eV	0.815 um
1	1.7616 eV	0.704 um

Band-Gap and Wavelength Dependence of Imaginary Refractive Index on X-Composition are tabulated at the values opposite and are extrapolated for other intermediate value.



## CIGS X-Composition (Band-Gap) Effects

- Effect of X-Composition (Band-Gap) on Spectral Response

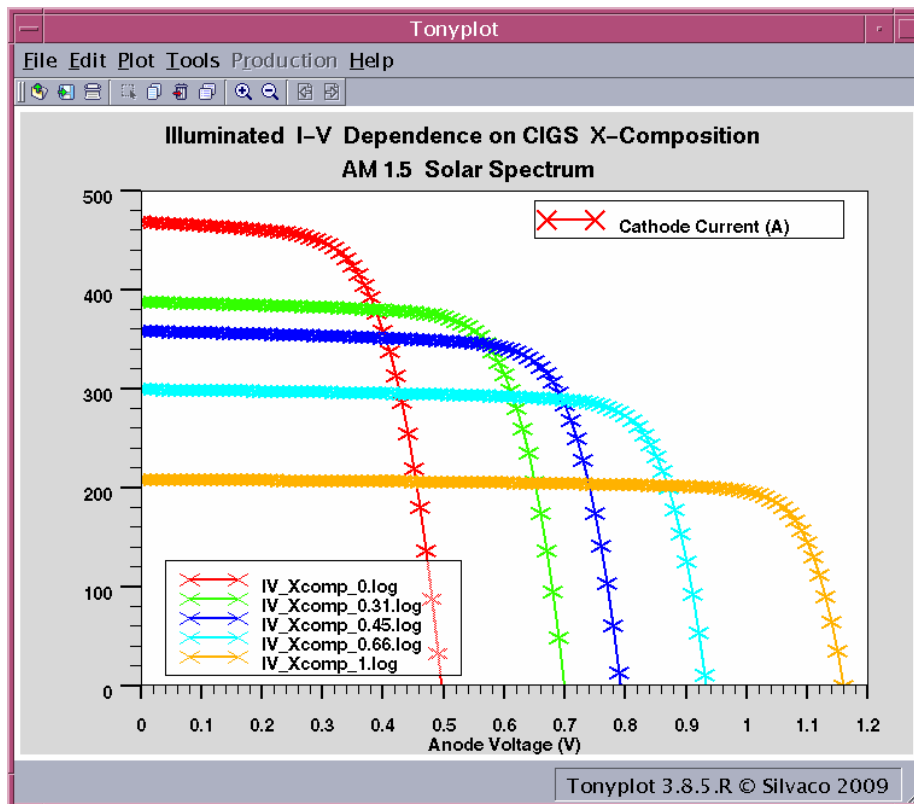


Increasing Band-Gap significantly reduces conversion efficiency at longer wavelengths, reducing current output.



# CIGS X-Composition (Band-Gap) Effects

- Illuminated I-V Curves for Different CIGS X-Composition

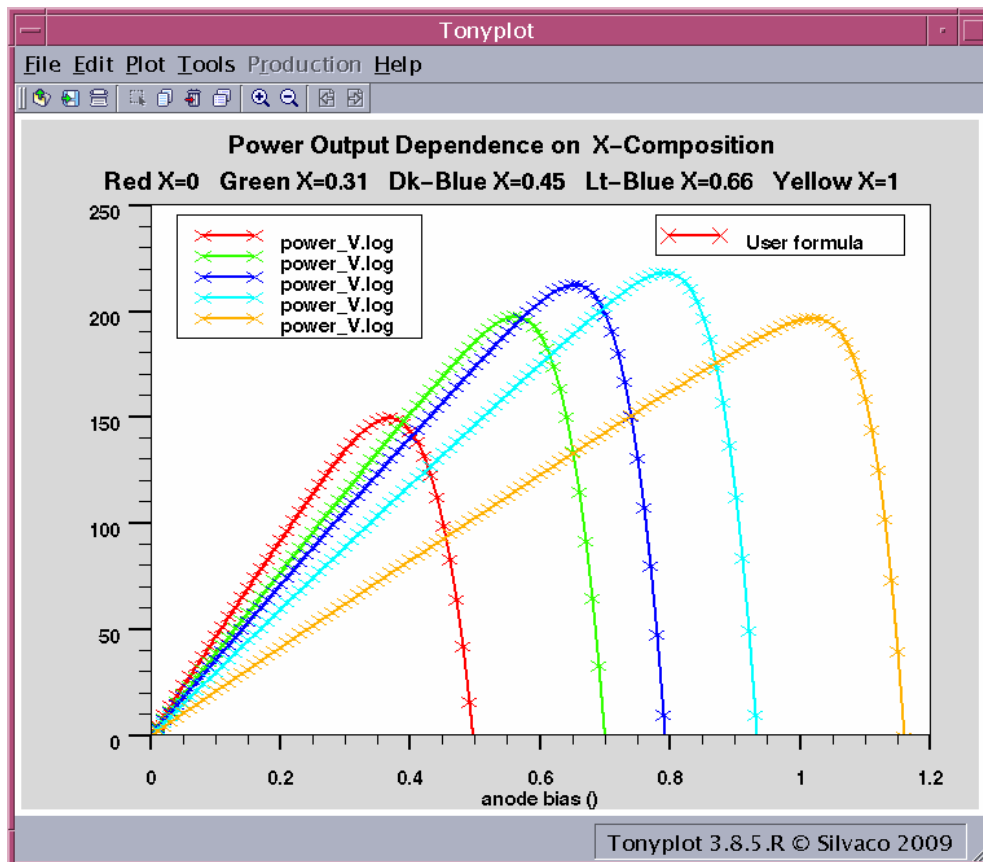


Output Current is significantly reduced, but Output Voltage increases



## CIGS X-Composition (Band-Gap) Effects

- Effect of X-Composition on Power Output



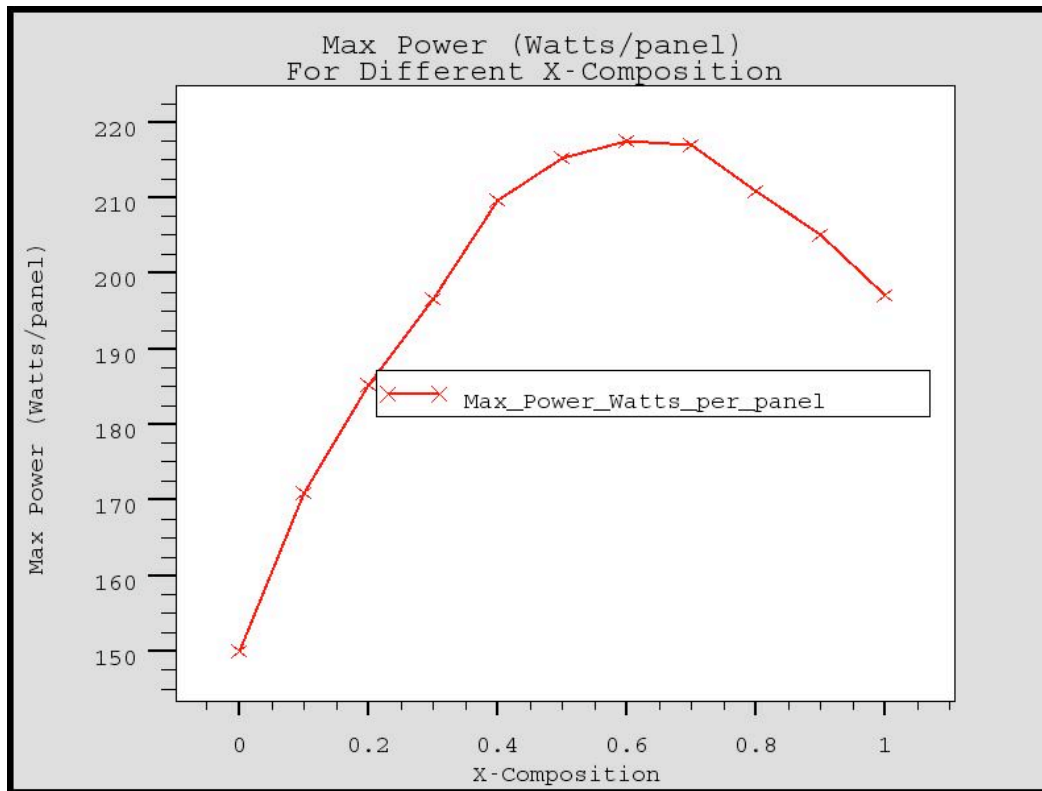
Output Power is Increased Dramatically using Larger Band-Gaps.

Optimum X-Composition is approximately X=0.66.



## CIGS X-Composition (Band-Gap) Effects

- Output from running VWF Experiments



Max Power Output  
versus X-Composition.

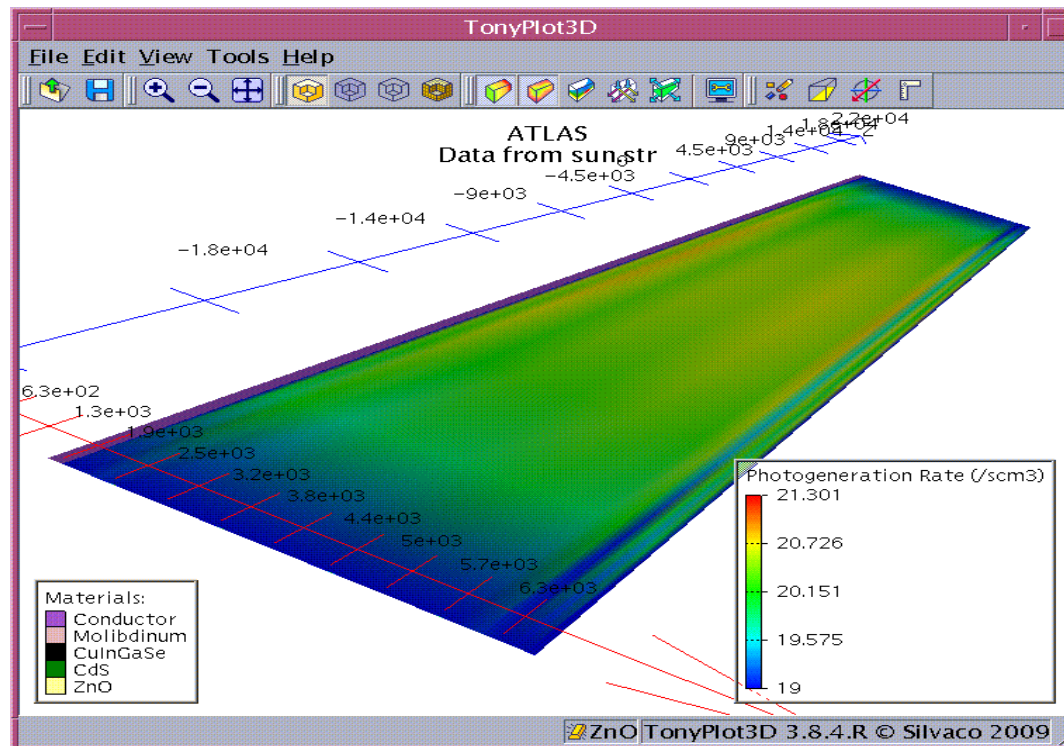
Peak Power for a Ga  
Fraction of 0.6.

Max Power increased  
by 43%.



## 3D Light Intensity Variation Effects

- Showing Surface Photo-generation Rate per Mesh Point on the surface of the 3D Simulated Solar Cell Structure

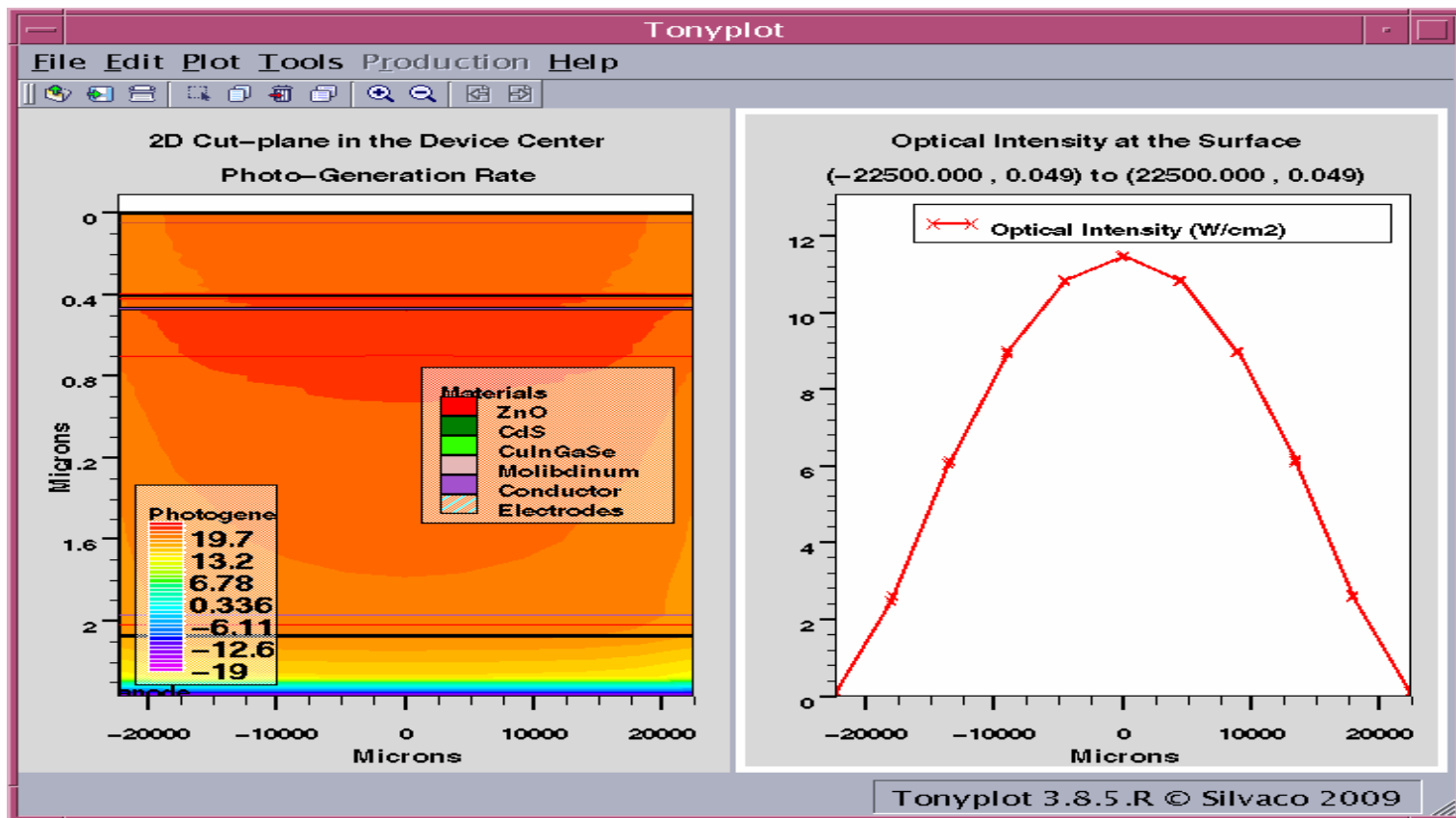


Apparent Striations in the X-Direction are a result of non-uniform meshing in this direction. It is actually plotting photo-generation per mesh point.



## 3D Light Intensity Variation Effects

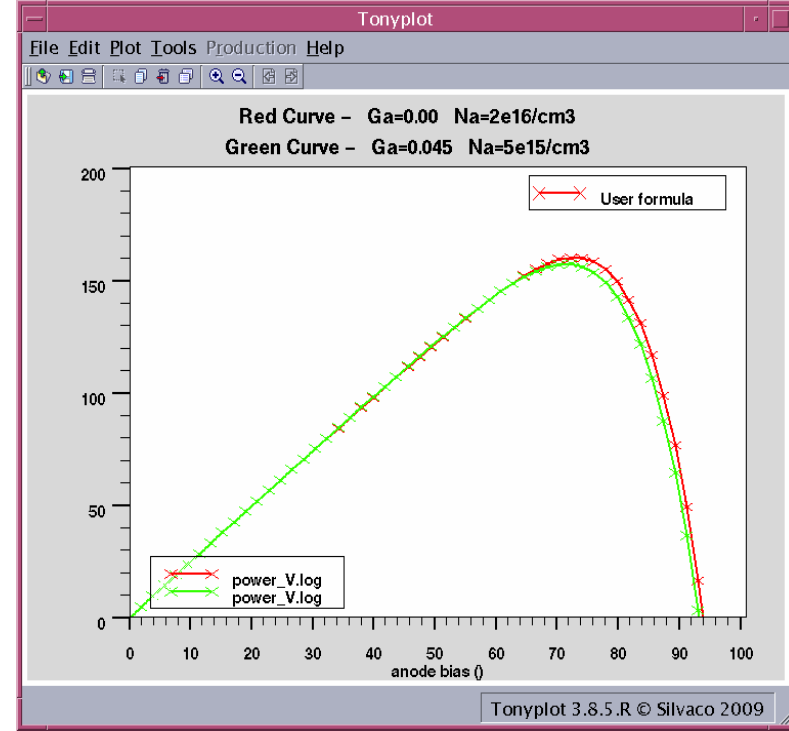
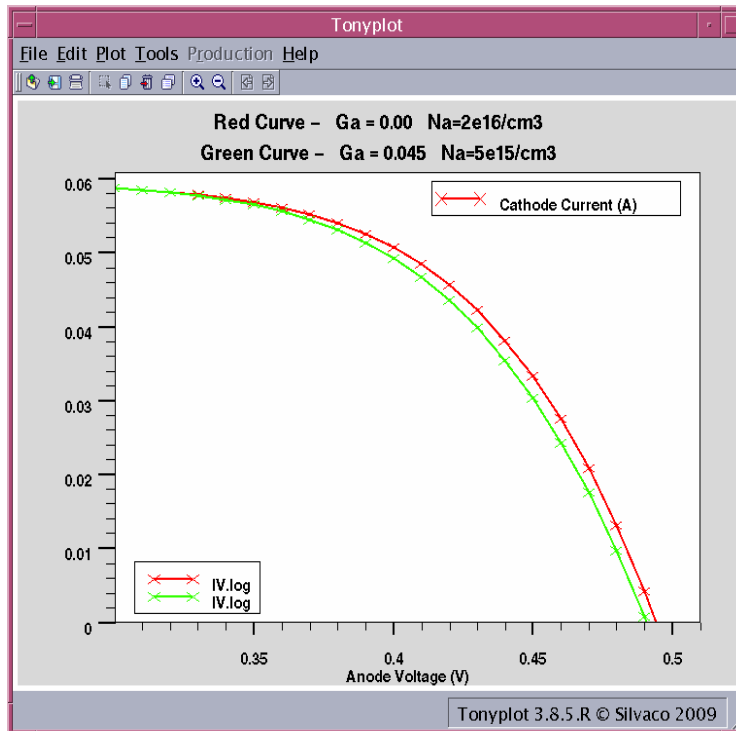
- A 2D Cut-Line Through the Center of the Solar Cell





## 3D Light Intensity Variation Effects

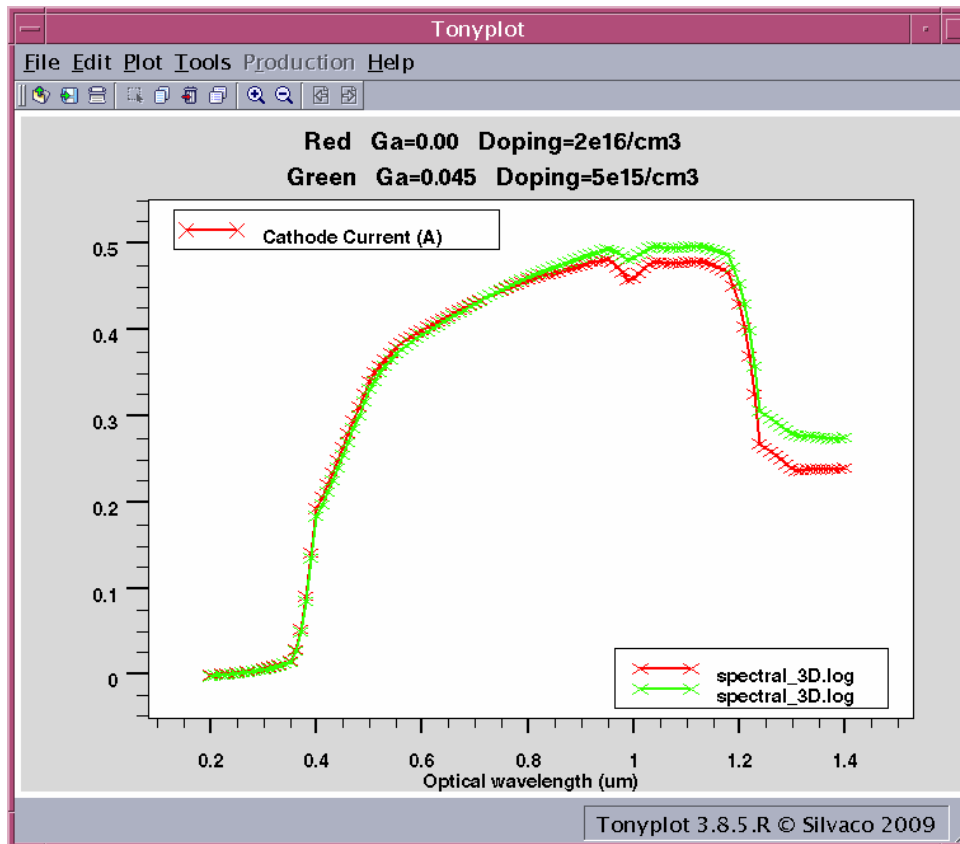
- Showing there is little difference between Increased Doping and Increased Band-gap with Lower Doping





## 3D Light Intensity Variation Effects

- Spectral Response of the two 3D Experiments



Larger  $E_g$  low doped material has better short wavelength response while smaller  $E_g$  higher doped material has better longer wavelength response. These two effects almost cancel out.



# Optimize the Solar Cell using VWF

SPAYN

File Edit View Tools Simulation Help

	ZnO_thk	CdS_thk	doping	x_comp	bandgap	max_lamb	Temperatu	Short_Circ	Op
1	1.150e+00	2.750e-01	1.000e+17	5.000e-01	1.410e+00	8.793e-01	4.500e+01	2.697e+02	8.7
2	1.150e+00	2.750e-01	1.000e+16	0.000e+00	1.069e+00	1.160e+00	4.500e+01	4.201e+02	4.9
3	1.150e+00	2.750e-01	1.000e+16	5.000e-01	1.410e+00	8.793e-01	4.500e+01	2.985e+02	8.2
4	1.150e+00	2.750e-01	1.000e+16	1.000e+00	1.761e+00	7.041e-01	4.500e+01	1.653e+02	1.15
5	1.150e+00	2.750e-01	5.050e+17	0.000e+00	1.069e+00	1.160e+00	4.500e+01	3.459e+02	5.8
6	1.150e+00	2.750e-01	5.050e+17	5.000e-01	1.410e+00	8.793e-01	4.500e+01	2.485e+02	9.2
7	1.150e+00	2.750e-01	5.050e+17	1.000e+00	1.761e+00	7.041e-01	4.500e+01	1.390e+02	1.25
8	1.150e+00	2.750e-01	1.000e+18	0.000e+00	1.069e+00	1.160e+00	4.500e+01	3.316e+02	6.1
9	1.150e+00	2.750e-01	1.000e+18	5.000e-01	1.410e+00	8.793e-01	4.500e+01	2.415e+02	9.4
10	1.150e+00	2.750e-01	1.000e+18	1.000e+00	1.761e+00	7.041e-01	4.500e+01	1.352e+02	1.27
11	1.150e+00	5.000e-02	1.000e+16	0.000e+00	1.069e+00	1.160e+00	4.500e+01	4.678e+02	4.9
12	1.150e+00	5.000e-02	1.000e+16	5.000e-01	1.410e+00	8.793e-01	4.500e+01	3.434e+02	8.2
13	1.150e+00	5.000e-02	1.000e+16	1.000e+00	1.761e+00	7.041e-01	4.500e+01	2.091e+02	1.16
14	1.150e+00	5.000e-02	5.050e+17	0.000e+00	1.069e+00	1.160e+00	4.500e+01	3.948e+02	5.9
15	1.150e+00	5.000e-02	5.050e+17	5.000e-01	1.410e+00	8.793e-01	4.500e+01	2.951e+02	9.3
16	1.150e+00	5.000e-02	5.050e+17	1.000e+00	1.761e+00	7.041e-01	4.500e+01	1.844e+02	1.27
17	1.150e+00	5.000e-02	1.000e+18	0.000e+00	1.069e+00	1.160e+00	4.500e+01	3.842e+02	6.2
18	1.150e+00	5.000e-02	1.000e+18	5.000e-01	1.410e+00	8.793e-01	4.500e+01	2.896e+02	9.6
19	1.150e+00	5.000e-02	1.000e+18	1.000e+00	1.761e+00	7.041e-01	4.500e+01	1.824e+02	1.30
20	1.150e+00	5.000e-01	1.000e+16	0.000e+00	1.069e+00	1.160e+00	4.500e+01	3.963e+02	4.8
21	1.150e+00	5.000e-01	1.000e+16	5.000e-01	1.410e+00	8.793e-01	4.500e+01	2.758e+02	8.1
22	1.150e+00	5.000e-01	1.000e+16	1.000e+00	1.761e+00	7.041e-01	4.500e+01	1.466e+02	1.14
23	1.150e+00	5.000e-01	5.050e+17	0.000e+00	1.069e+00	1.160e+00	4.500e+01	3.238e+02	5.8
24	1.150e+00	5.000e-01	5.050e+17	5.000e-01	1.410e+00	8.793e-01	4.500e+01	2.273e+02	9.1
25	1.150e+00	5.000e-01	5.050e+17	1.000e+00	1.761e+00	7.041e-01	4.500e+01	1.214e+02	1.25
26	1.150e+00	5.000e-01	1.000e+18	0.000e+00	1.069e+00	1.160e+00	4.500e+01	3.087e+02	6.0
27	1.150e+00	5.000e-01	1.000e+18	5.000e-01	1.410e+00	8.793e-01	4.500e+01	2.206e+02	9.3
28	1.150e+00	5.000e-01	1.000e+18	1.000e+00	1.761e+00	7.041e-01	4.500e+01	1.177e+02	1.27
29	3.000e-01	5.000e-02	1.000e+16	0.000e+00	1.069e+00	1.160e+00	4.500e+01	4.798e+02	4.9
30	3.000e-01	5.000e-02	1.000e+16	5.000e-01	1.410e+00	8.793e-01	4.500e+01	3.534e+02	8.2
31	3.000e-01	5.000e-02	1.000e+16	1.000e+00	1.761e+00	7.041e-01	4.500e+01	2.180e+02	1.16

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- First, Simulate all the Experiments
- The integrated statistical package called SPAYN loads all the results into it's data base.



# Optimize the Solar Cell using VWF

**Parameters**

- Max\_Panel\_Current
- Max\_Panel\_Voltage
- Pmax\_Panel\_Current
- Pmax\_Panel\_Voltage
- Max\_Power\_Watts\_per\_panel

**Predictors**

- ZnO\_thk
- CdS\_thk
- doping
- x\_comp

**Targets**

- Conversion\_Effi...

**Regression Terms**

- Linear (x)
- Interactions (xy)
- Quadratic (x<sup>2</sup>)
- Interactions (xyz)
- Interactions (x<sup>2</sup>y)
- Cubic (x<sup>3</sup>)

**Solve**

Show Coeffs.    Fit Info.    Scatter Plot.

**Regression Model for Selected Target**

Conversion\_Efficiency =

$$8.345e-02 + 8.452e-04*(ZnO\_thk - 1.150e+00) - 6.335e-02*(CdS\_thk - 2.750e-01) - 3.382e-20*(doping - 5.001e+17) + 1.245e-02*(x\_comp - 5.000e-01)$$

**Fit Error / ANOVA Information for Selected Target**

FIT ERRORS:

	MEAN	MAXIMUM
RELATIVE	5.07%	-18.82%
ABSOLUTE	3.018E-03	9.911E-03

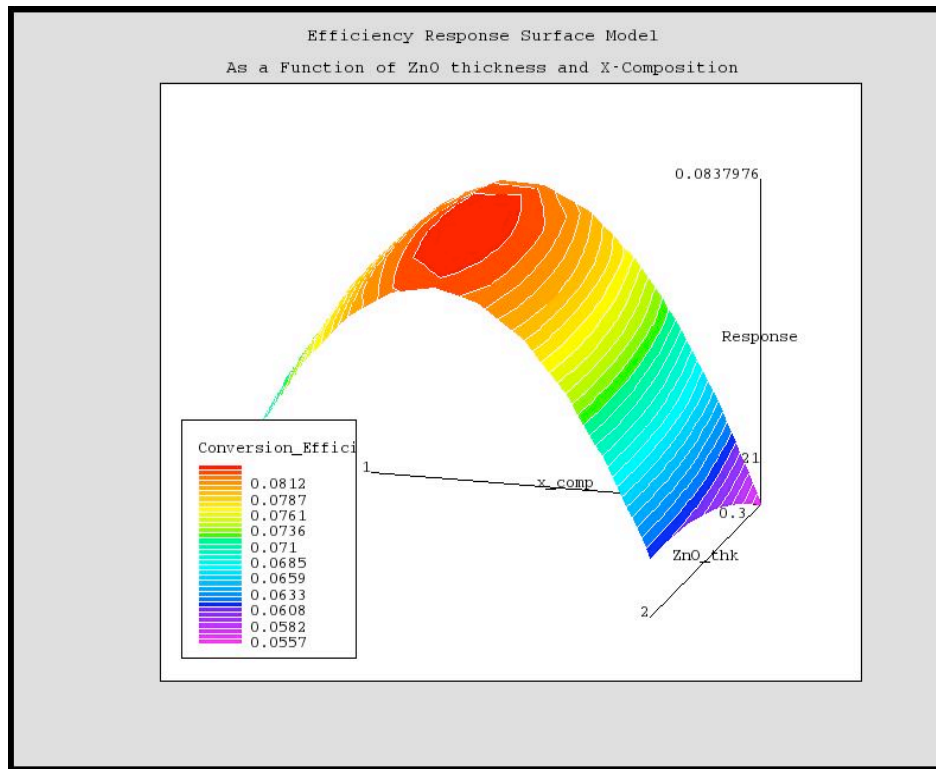
ANALYSIS OF VARIANCE:

- Click “Tools... Regression” to create a Response Surface Model (R.S.M.)
- Choose a “Target” and “Input Parameters” to create the model



## Optimize the Solar Cell using VWF

- Click TonyPlot to Visualize Response Surface Models



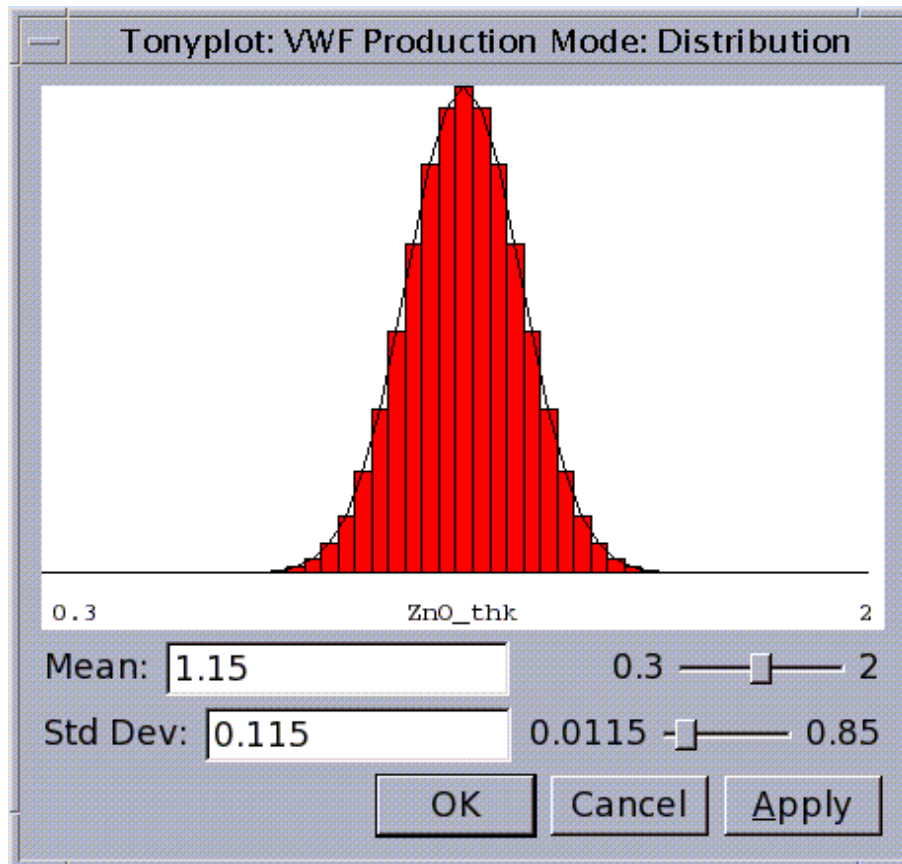
This example shows the Solar Cell Efficiency “Response Surface” using the two variables ZnO thickness and X-Composition.

This makes it simple to read off optimum values for cell efficiency.



## Optimize the Solar Cell using VWF

- Effects of ZnO Thickness Variation during Production Runs



In this example, we analyze the effects of ZnO thickness variation during production.

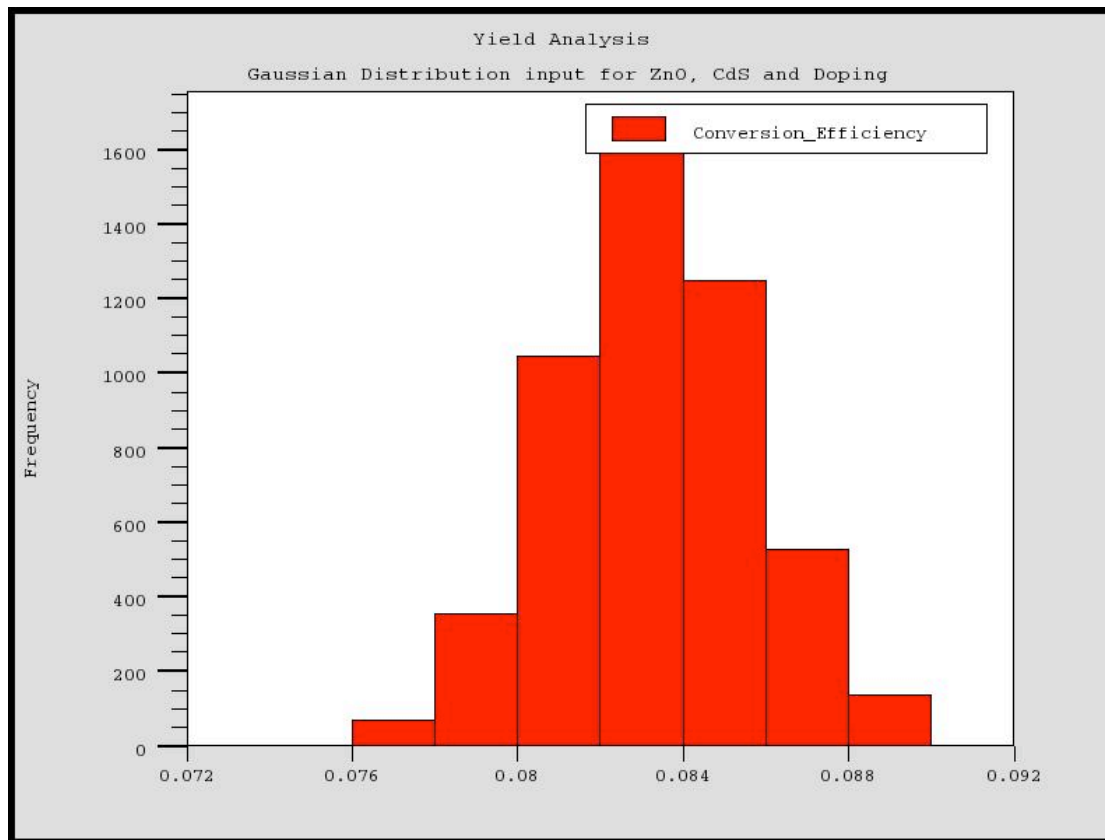
A “Gaussian” thickness variation is input into the model.

We can instantly see the effects on the solar cell output.



# Optimize the Solar Cell using VWF

## ■ Results of Production Thickness Variations

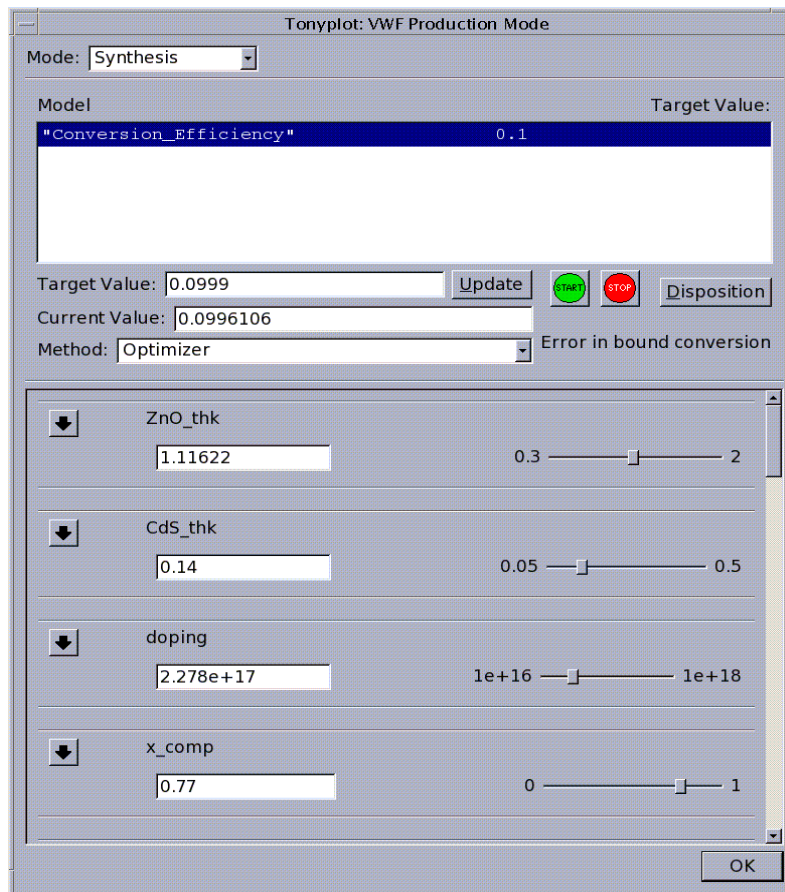


Here we analyze the effects of thickness variations on Solar cell efficiency.



# Optimizing the Solar Cell using VWF

## ■ Optimized Parameters



Optimized Parameters for all 4 variables from the Response Surface Model (RSM) created by VWF's integrated statistical package called SPAYN, for a required solar cell overall efficiency of 10% that is requested by the user.



## Conclusions

- The Response Surface Model created by the VWF environment gave good agreement with the individually simulated structures, validating this approach to global device optimization
- Increasing ZnO Thickness increases Power Output by 8 Watts per Panel. The extra absorption in the thicker ZnO layer is more than made up for by reduced electrical losses
- The CdS Thickness seems near optimal. Basically the thinner the better, but not fully depleted
- Increased Doping in the CIGS layer increases output power mainly due to Increased Output Voltage
- Increasing Bandgap Increases Maximum Output Power due to increased output voltage (but Output Current is reduced)