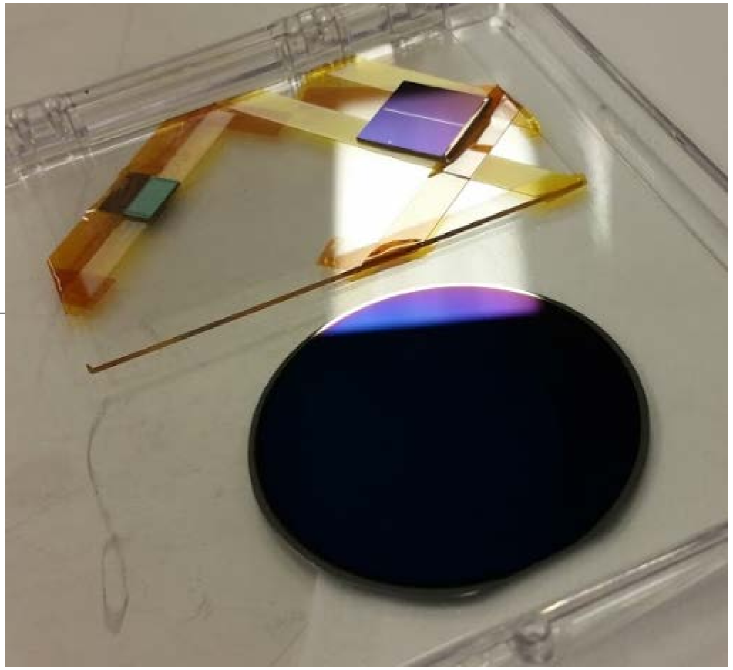
35^{th} Annual Microelectronic Engineering Conference 2017:

MgF_2-Ta_2O_5 Anti Reflective Coating for 3^{rd} Generation Solar Cells



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Project Scope

1. Develop a mathematical model to optimize MgF_2-Ta_2O_5 bi-layer anti-reflective coatings (ARCs).
2. Deposit the ARC on silicon substrates and test broad band reflectivity.
3. Measure the diffuse field reflectance of ARC.
4. Show an improvement in solar cell performance for a solar cell with the ARC verses without.

Theory behind the Simulation Model

The method of resultant waves was applied in MATLAB to make iterative calculations in order to determine the film thickness combinations that result in the lowest average reflectivity.

Boundary Conditions

$$r_{i-1} = \frac{n_{i-1} - n_i}{n_{i-1} + n_i} \quad t_{i-1} = 1 - r_{i-1} \quad \delta_i = \frac{2\pi d_i n_i}{\lambda} \quad E_+^i = \frac{E_+^{i+1} + r_i E_-^{i+1}}{t_i} \quad E_-^i = \frac{r_i E_+^{i+1} + E_-^{i+1}}{t_i}$$

$$n_0 | n_1 | n_2 | n_g = n_{air} | n(\lambda)_{MgF_2} | n(\lambda)_{Ta_2O_5} | n(\lambda)_{Si}$$

Electric Field for m Dielectric Films

$$\boldsymbol{I_i} = \begin{bmatrix} \frac{1}{t_i} & \frac{r_i}{t_i} \\ \frac{r_i}{t_i} & \frac{1}{t_i} \end{bmatrix} \quad \boldsymbol{T_i} = \begin{bmatrix} e^{i\delta_i} & 0 \\ 0 & e^{-i\delta_i} \end{bmatrix}$$

$$\boldsymbol{M} = \boldsymbol{I_0} \times \boldsymbol{T_1} \times \boldsymbol{I_1} \times \boldsymbol{T_2} \times \cdots \times \boldsymbol{I_{m-1}} \times \boldsymbol{T_m} \times \boldsymbol{I_m}$$

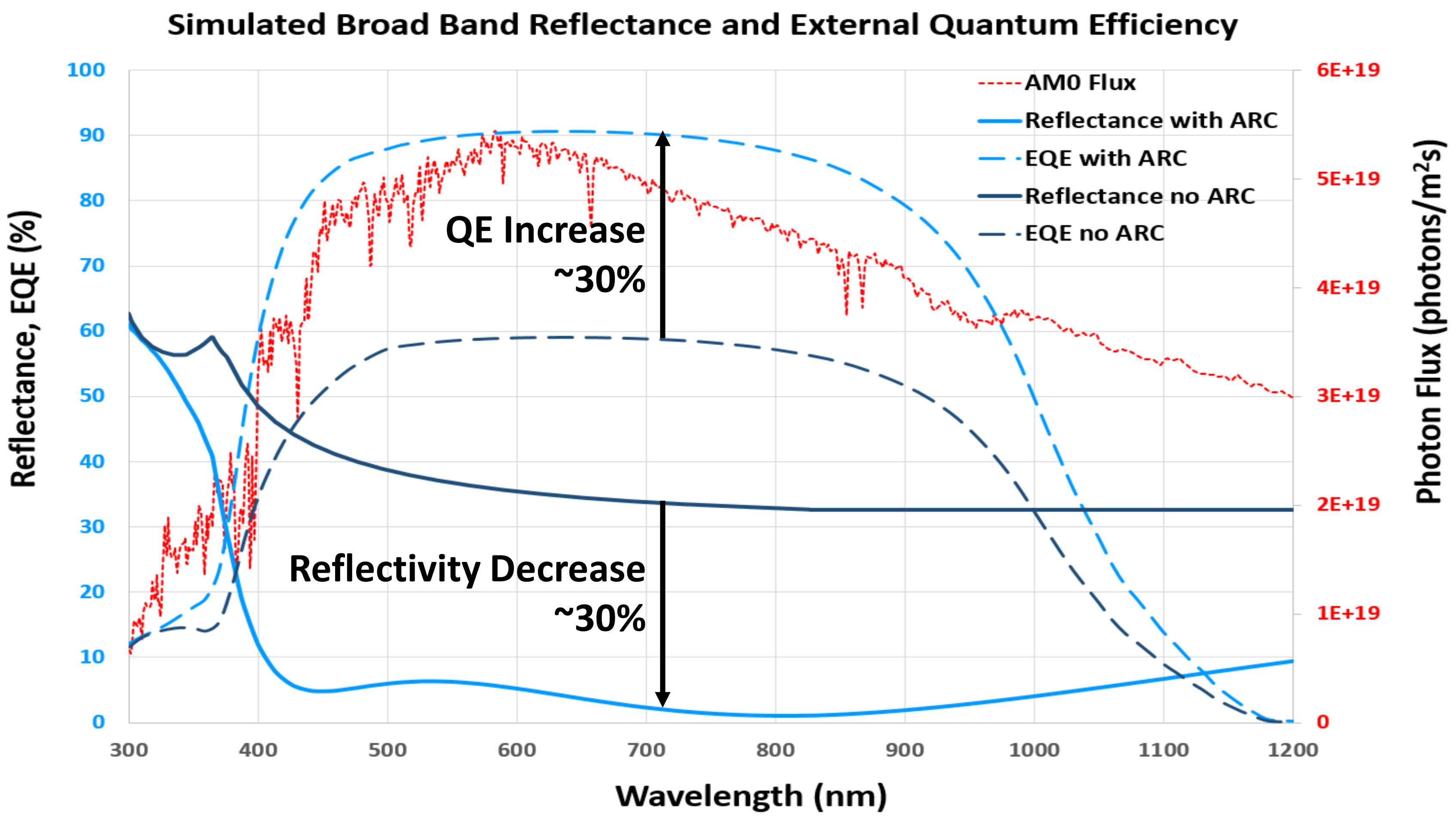
$$\begin{pmatrix} E_+^0 \\ E_-^0 \end{pmatrix} = \boldsymbol{M} \begin{pmatrix} E_+^f \\ E_-^f \end{pmatrix} \qquad \begin{pmatrix} E_+^f \\ E_-^f \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Average Broad Band Reflectivity

$$\rho = \frac{E_-^0}{E_+^0} \quad R(\lambda) = |\rho||\rho^*| \quad AM0\ Flux = F(\lambda) \quad R_e = \frac{\int_{\lambda_1}^{\lambda_2} F(\lambda) R(\lambda) d\,\lambda}{\int_{\lambda_1}^{\lambda_2} F(\lambda) d\,\lambda}$$

λ – wavelength
n – Complex index of refraction as a function of λ
r – Reflectance Fresnel coefficient
t – Transmission Fresnel coefficient
δ – Change in phase of light through a medium
d – Stack layer thickness
E^+ – Transmitted component of the light's electric field
E^- – Reflected component of the light's electric field
ρ – Stack reflectance coefficient
R_e – Average stack reflectivity for a range of λ

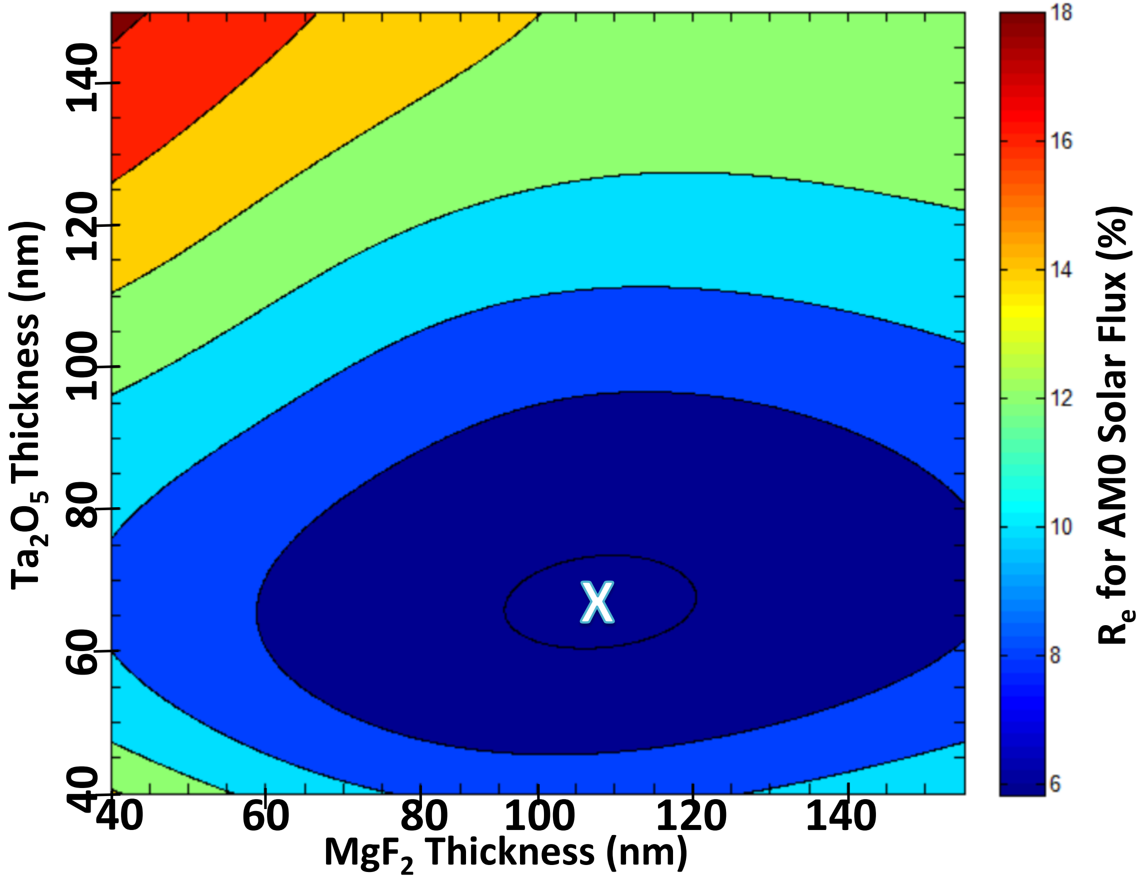
Reflectivity and Quantum Efficiency Curves



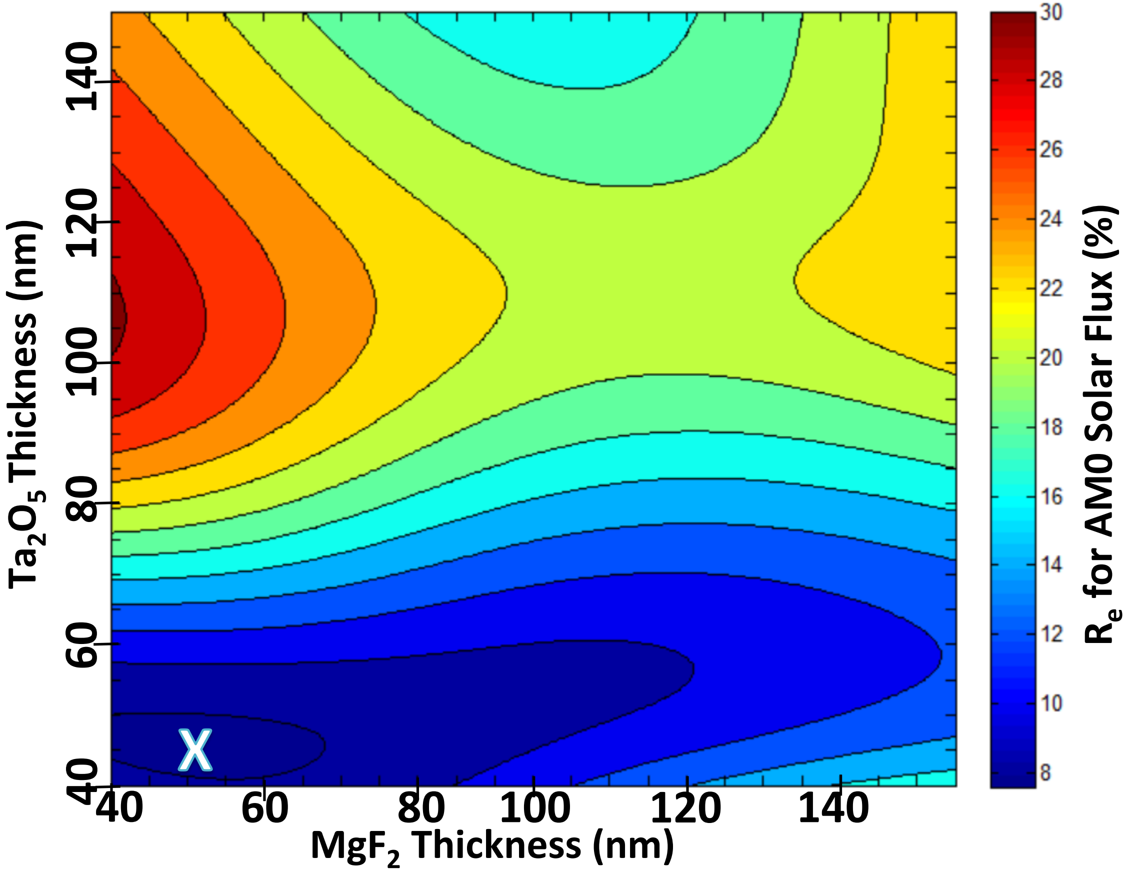
- ❖ AM0 flux data is referenced from NREL
- ❖ Reflectivity curves were generated in MATLAB
- ❖ EQE curves were generated in PC1D where the simulated reflectivity data was imported.

MgF_2-Ta_2O_5 Bi-layer
Broad Band Reflectance Contour Plots

For Wavelengths between 300 – 1200 nm



For Wavelengths between 400 –700 nm



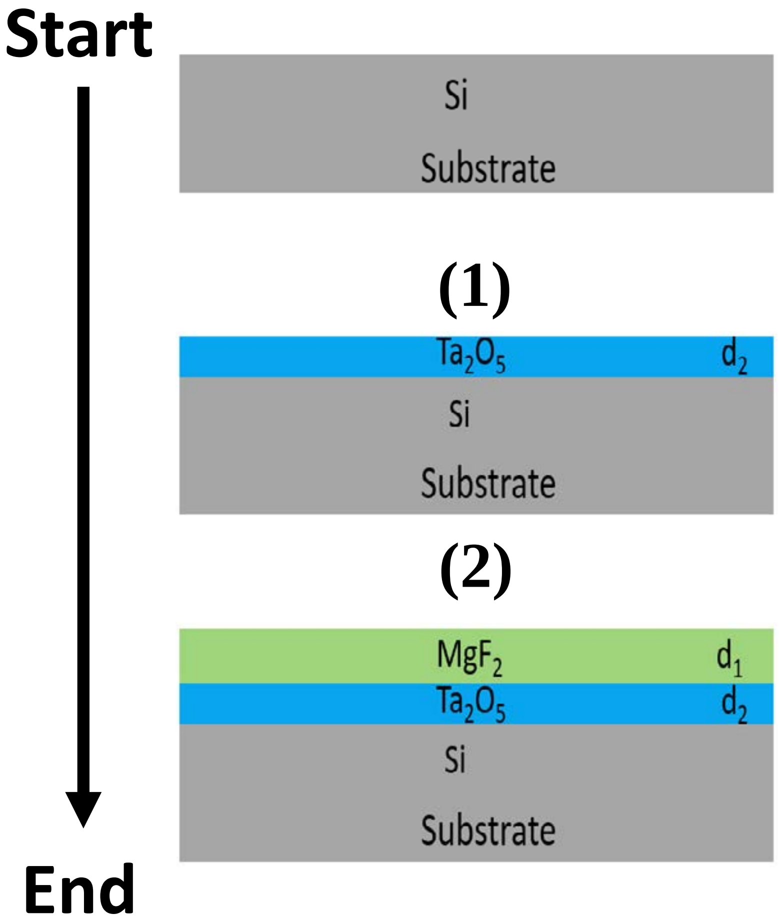
ARC Deposition Process

(1) Ta_2O_5 Reactive Sputter in CVC601

- 4” Tantalum target
- Base Pressure 5 mTorr
- 33% O2 to Ar gas mixture
- 400W DC Power during deposition
- Deposition rate ~6 Å/s
- 117 second DC sputter
- Target thickness 70 nm

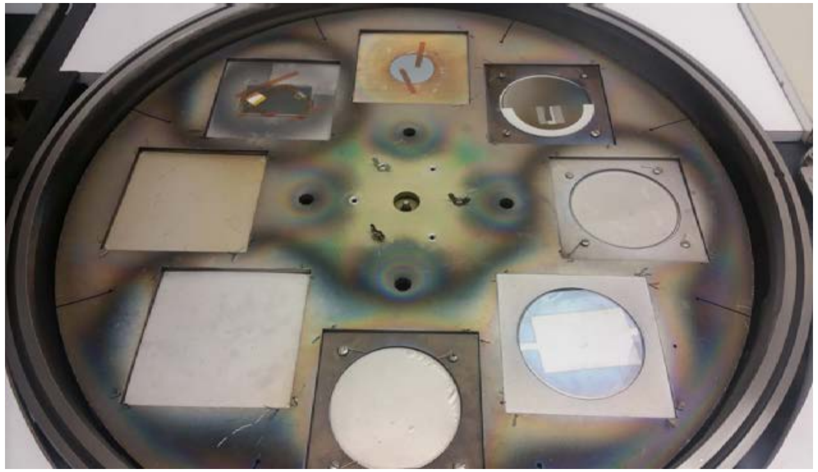
(2) MgF_2 Thermal Evaporation in PVD75A

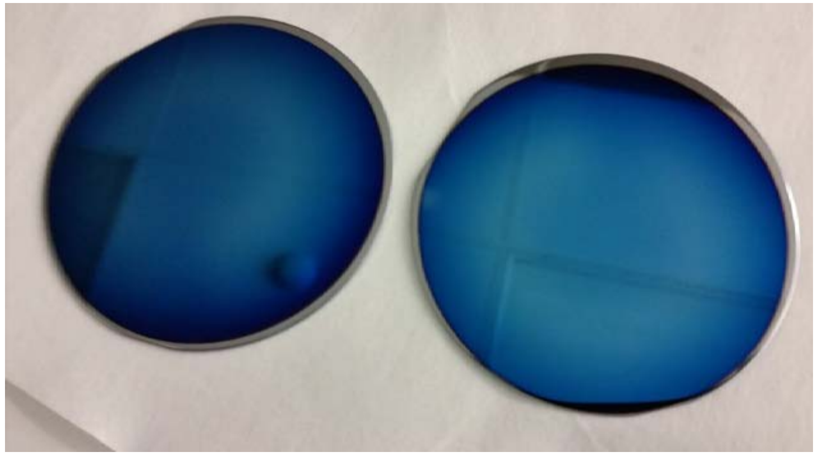
- MgF_2 crystals loaded in Mo boat
- Followed Brittany Smith’s process
- Spacers added under samples to minimize the effect of bloom adding to thickness non uniformity
- Deposition rate ~3-4 Å/s at 95% source power
- Target thickness 105 nm or 0.105 kÅ
- Reflectometry (Filmetrics Reflectometer) technique was used on a glass monitor slide to confirm thicknesses



Tantalum Oxide Reactive Sputter Findings

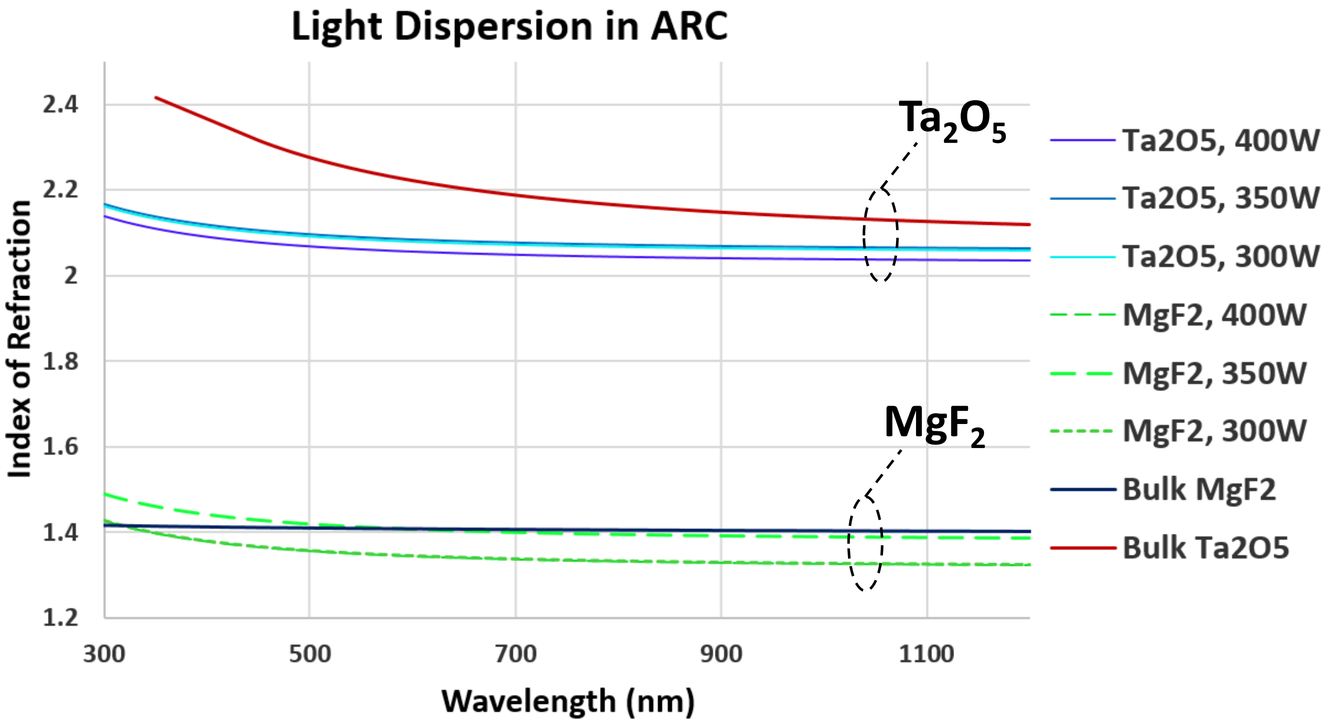
- DC sputter power 400W
  - Fastest deposition rate (~6 Å/s)
  - No sacrifice in index of refraction
  - Thickness uniformity showed negligible change
- Flow rates set to 9.3 ± 0.2 sccm
  - Replaces oxygen consumed during deposition
  - Resulted in less change in chamber pressure during deposition
- 33% Oxygen/Argon gas mixture
  - Results in higher oxygen content in the film
  - Lower oxygen content results in more absorbing film



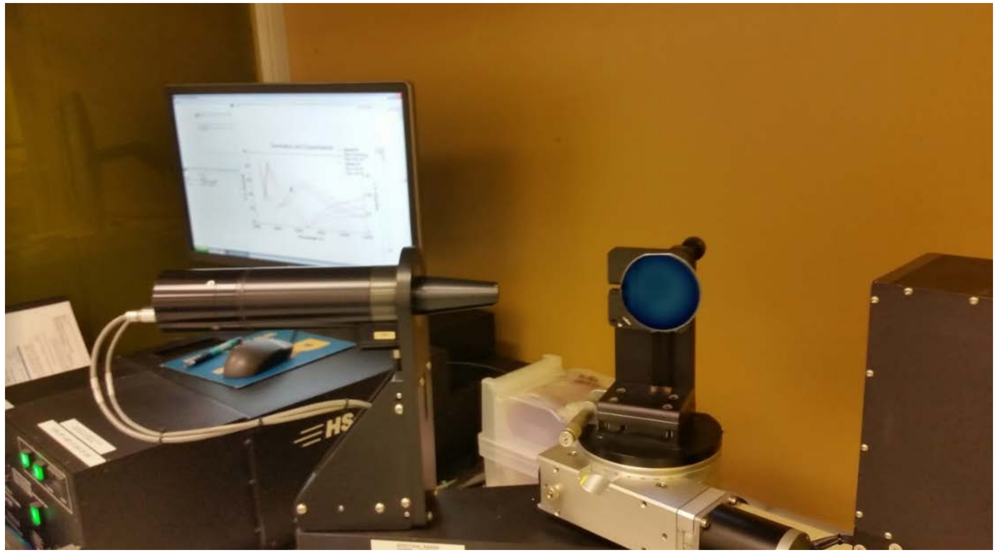


Measuring Index of Refraction

The light dispersion through each film material was investigated and experimentally measured using ellipsometry techniques. Each measured film was compared back to the bulk refractive properties found at RefractiveIndex.info.

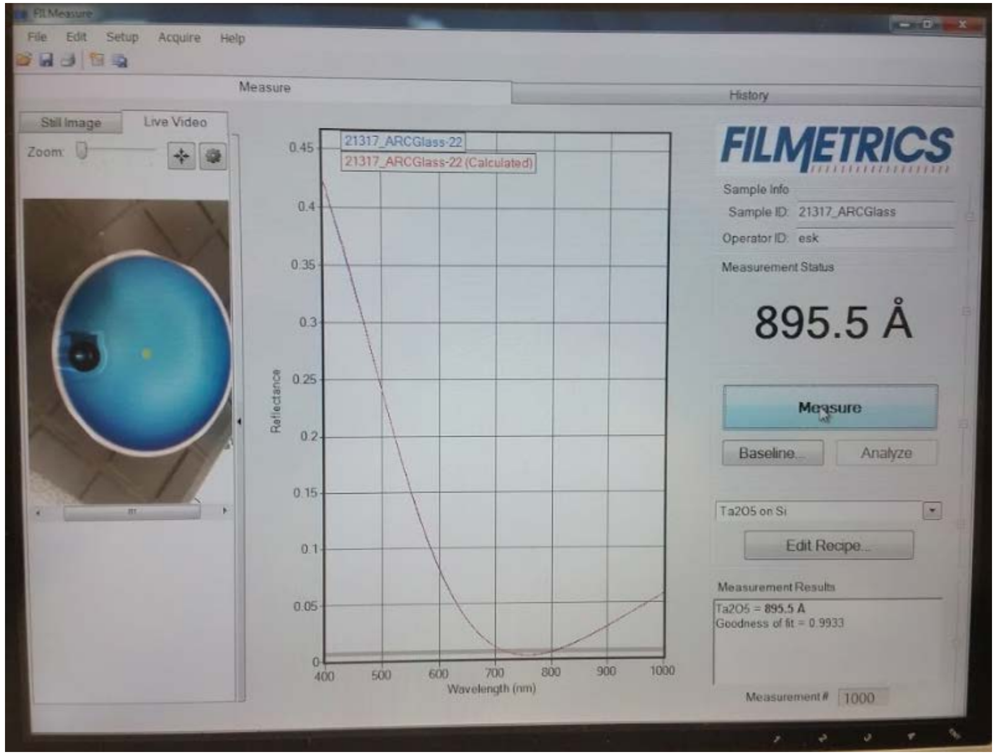


WVASE Setup

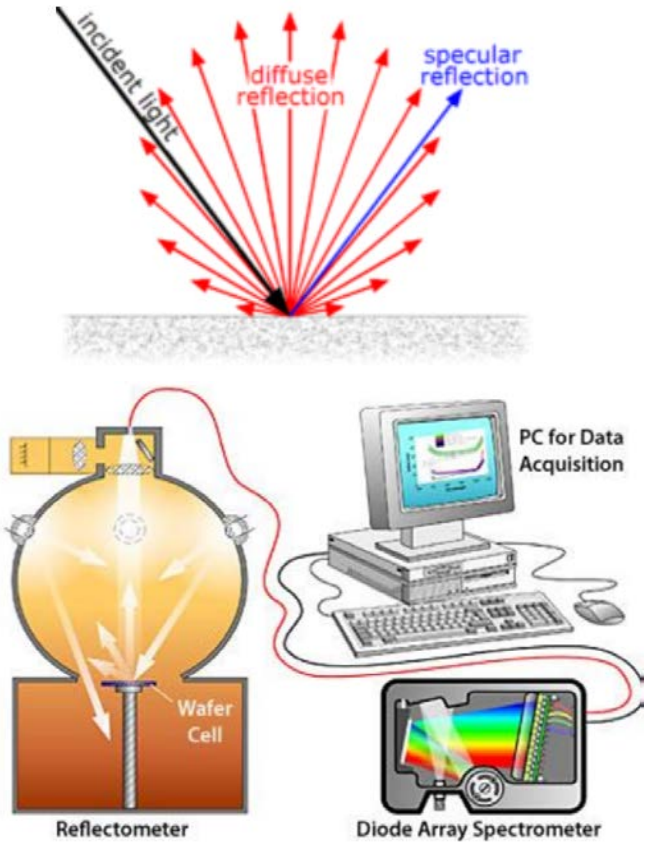


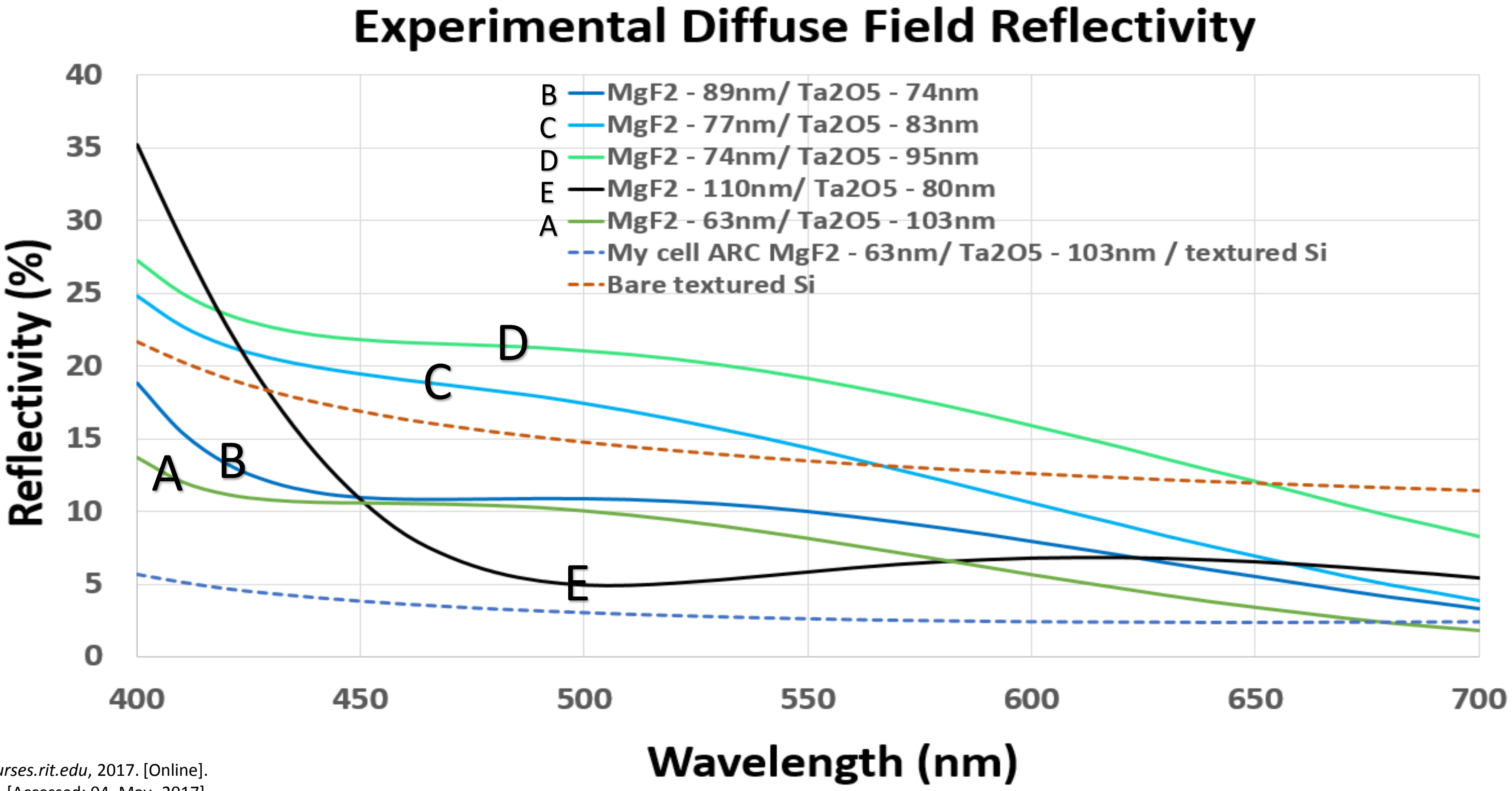
Measuring Film Thicknesses

- P2 Tencor Profilometer
  - Glass monitor slides bisected with kapton tape
  - Step heights measured from glass to substrate
- WVASE
  - Cauchy model was used for each material
  - Both index of refraction and thickness can be measured
  - Profilometer results used as baseline thicknesses
- Filmetrics Reflectometer
  - Used to originally measure MgF_2 on monitor slides
  - Imported Ta_2O_5 index data from WVASE
  - Much faster to use than both the WVASE and P2 Tencor



Reflectivity Measurements at the University of Rochester





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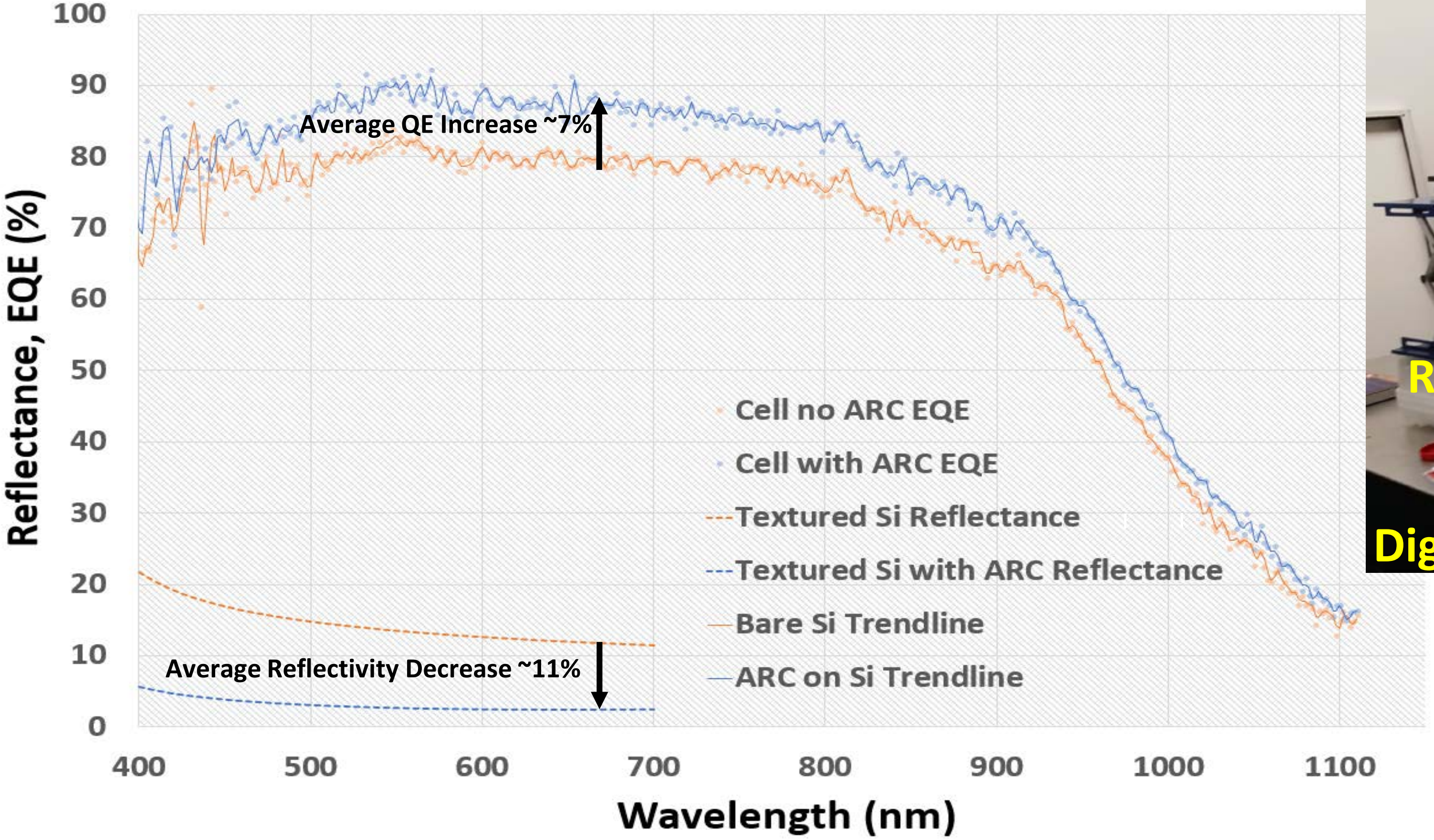
Simulated vs Experimental Average Reflectance

Sample ID (MgF_2-Ta_2O_5)	Simulated R_{avg} (%)	Simulated with 6nm Interfacial Oxide R_{avg} (%)	Experimental R_{avg} (%)
A (103nm-63nm)	5.4776	5.9951	7.2
B (89nm-74nm)	6.7757	8.9558	8.9
C (77nm-83nm)	10.4181	13.392	13.2
D (74nm-95nm)	15.0234	17.6412	17.4
E (110nm-80nm)	6.4863	8.1601	8.1
Textured Si cell no ARC	**-**	**-**	14.0
Textured Si cell with ARC 'A'	**-**	**-**	2.9

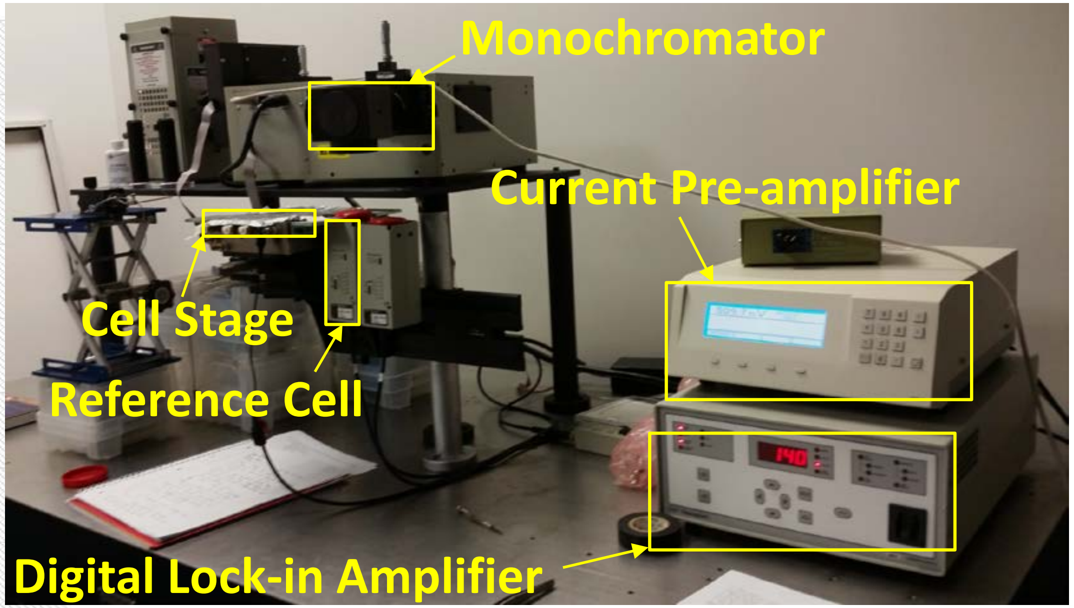
- Wafer samples for films **A** - **E** had a ~6nm thick native silicon oxide layer.
- Textured samples were chemically etched prior to depositing ARC.

Solar Cell Quantum Efficiency Measurements

Experimental Bi-layer ARC on c-Si Solar Cell



QE Experimental Setup



Conclusions and Future Work

- The bi-layer ARC design that resulted in the lowest average reflectivity under AM0 spectral irradiance was determined to be 105 nm of MgF_2 on top of 70 nm of Ta_2O_5 when mathematically modeled.
- Diffuse reflectance measurements of the bilayer film stacks followed the same trend as the proposed model for a variety of thickness combinations.
- MgF_2-Ta_2O_5 bi-layer ARC resulted in an average reflectivity decrease by 11% and increased the quantum efficiency by 7% in a commercial c-Si solar cell for wavelengths ranging from 400 nm to 700 nm.

Future Work

- Utilize e-beam evaporation and deposit on dynamic substrates
- Test ARC on III-V solar cells, and test designs for AM1.5 applications
- Integrate deposition process into existing cell fabrication at RIT
- Incorporate surface roughness into MATLAB model

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