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Covalent Metrology, Max Junda

CdS Bandgap Mapping by Spectroscopic Ellipsometry

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Statement of Work & Results Summary

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Goal: *Measurement of the spatial uniformity of the bandgap of a CdS thin film both before and after annealing.*

Methods: Mapping spectroscopic ellipsometry is collected in a 36-point grid across the full sample area before and after annealing.

Results Summary:

- The average bandgap energy is found to increase after annealing with the following averages:
  - Before Annealing: **2.23 eV**
  - After Annealing: **2.37 eV**
- The bandgap spatial uniformity is decreased following annealing.
- The increased surface roughness following annealing suggests grain growth as a result of the annealing process.
- Raw results data is provided alongside this report in spreadsheet format.

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Measurement Results

Mapped Bandgap Results

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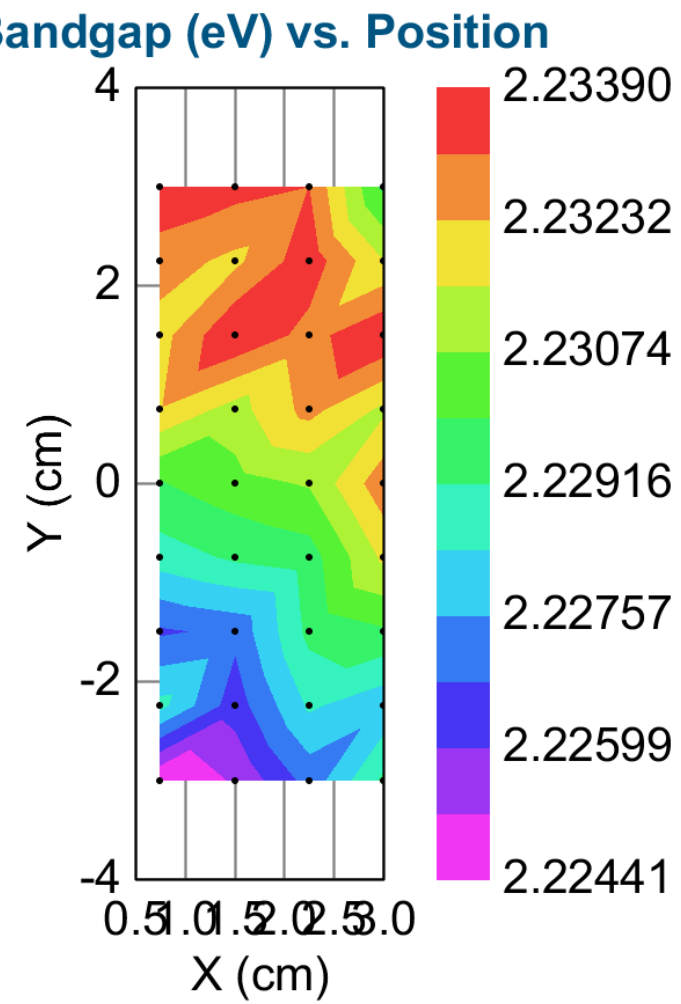
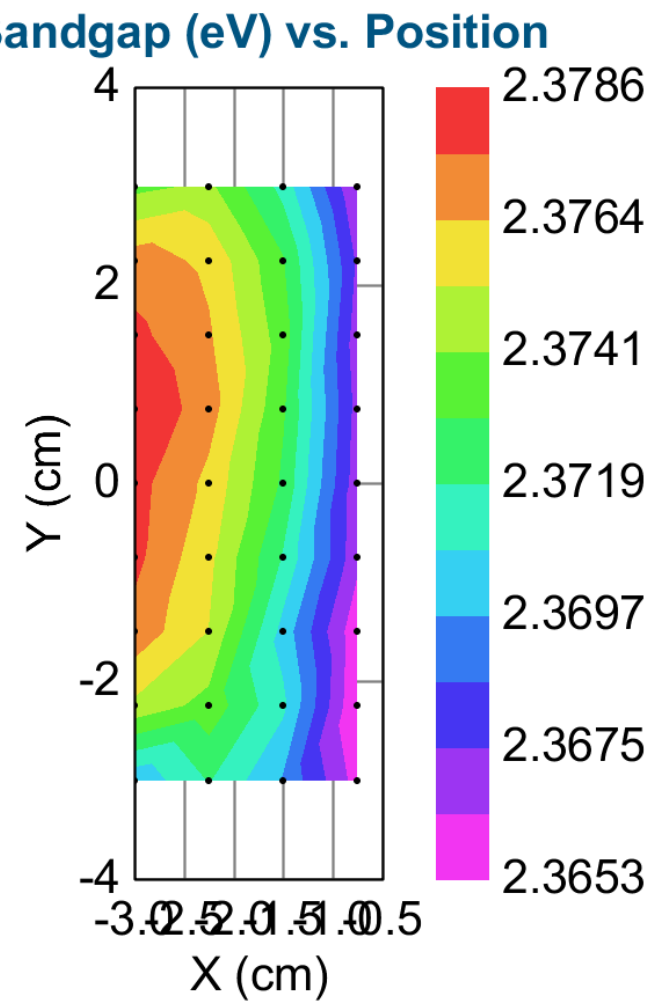
Before Anneal



After Anneal



Mapped MSE Results

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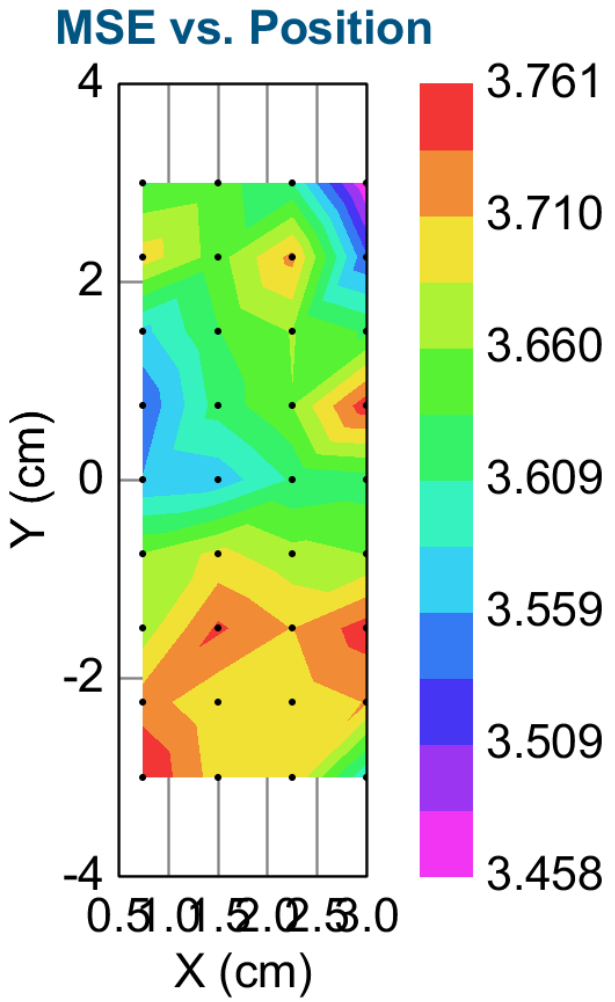
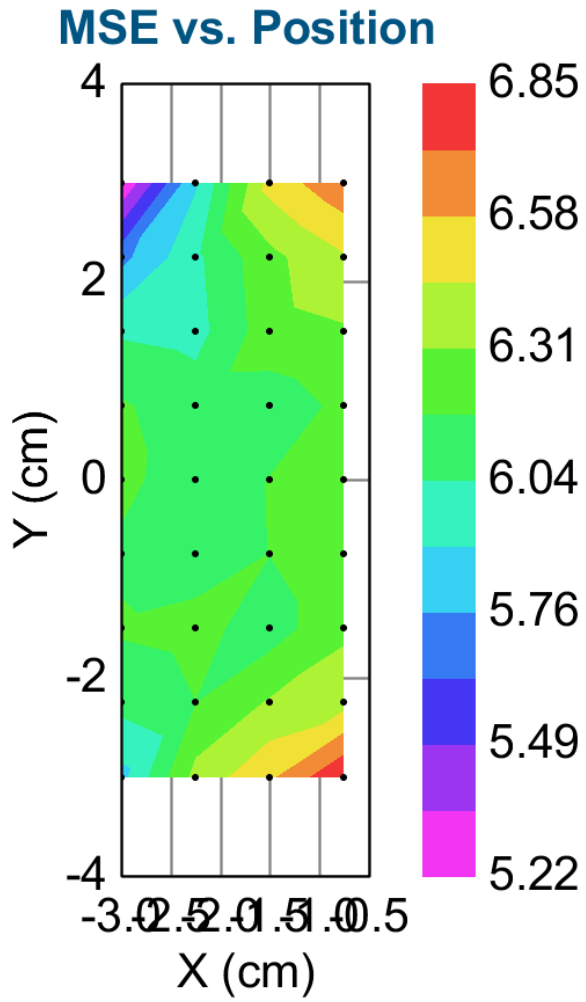
- The mean squared error function (MSE) is a relative measure of how well the model fits the measured data.
- It quantifies any mismatch between the model-generated and measured spectra such that lower MSE values correspond to better model fits.

Before Anneal



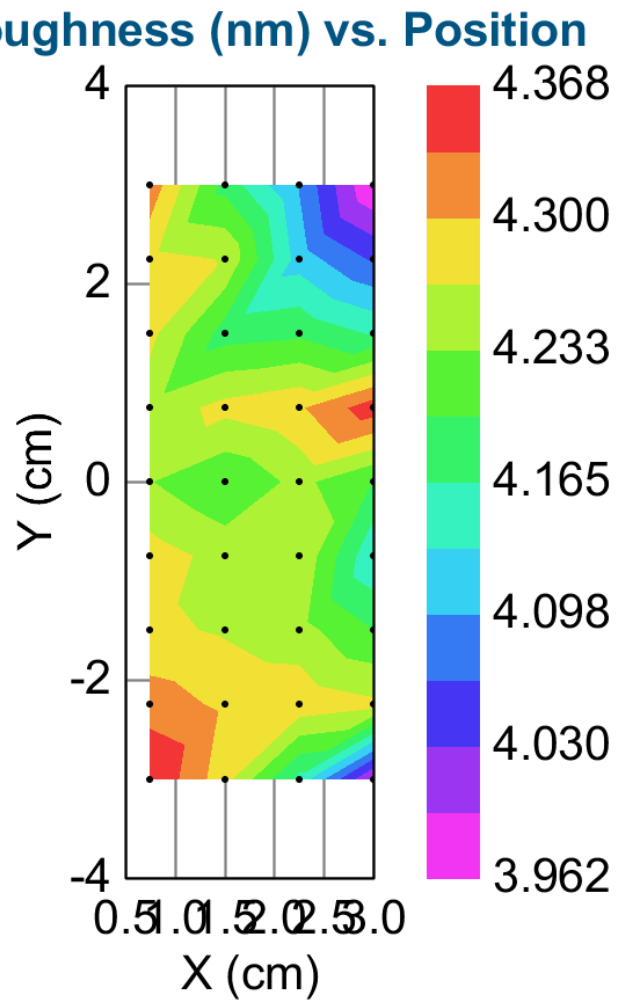
After Anneal



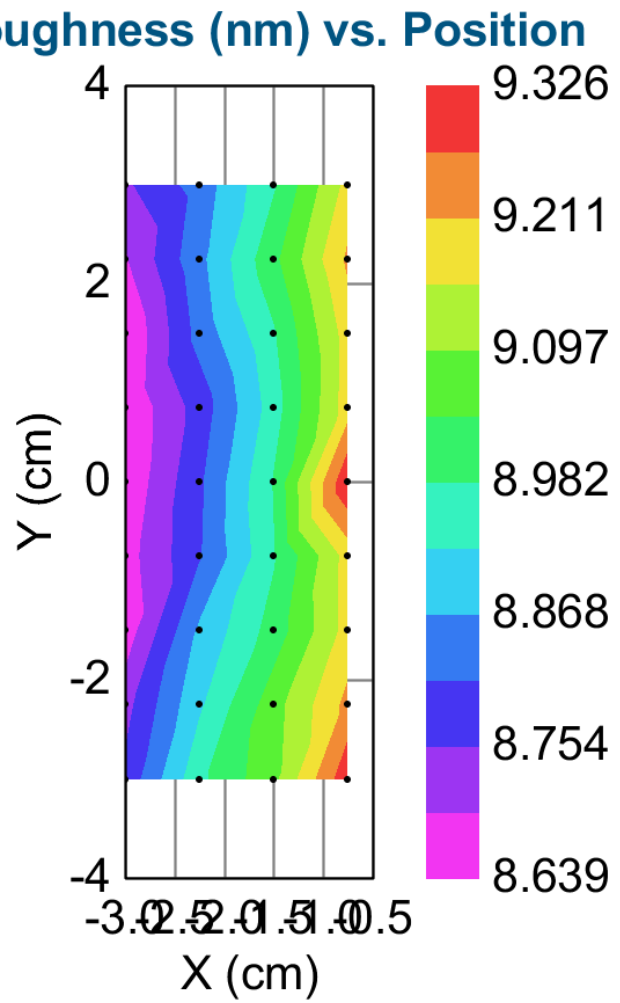
Mapped Surface Roughness Results

- The surface roughness of the film approximately doubles as a result of annealing.
- Generally, annealing is known to improve the crystallographic order in a material and promote the growth of larger grains.
- Increased surface roughness is consistent with larger grain size since larger individual grains protruding from the surface more.
- Additional characterization (such as XRD) would be required to confirm this grain size hypothesis with certainty.

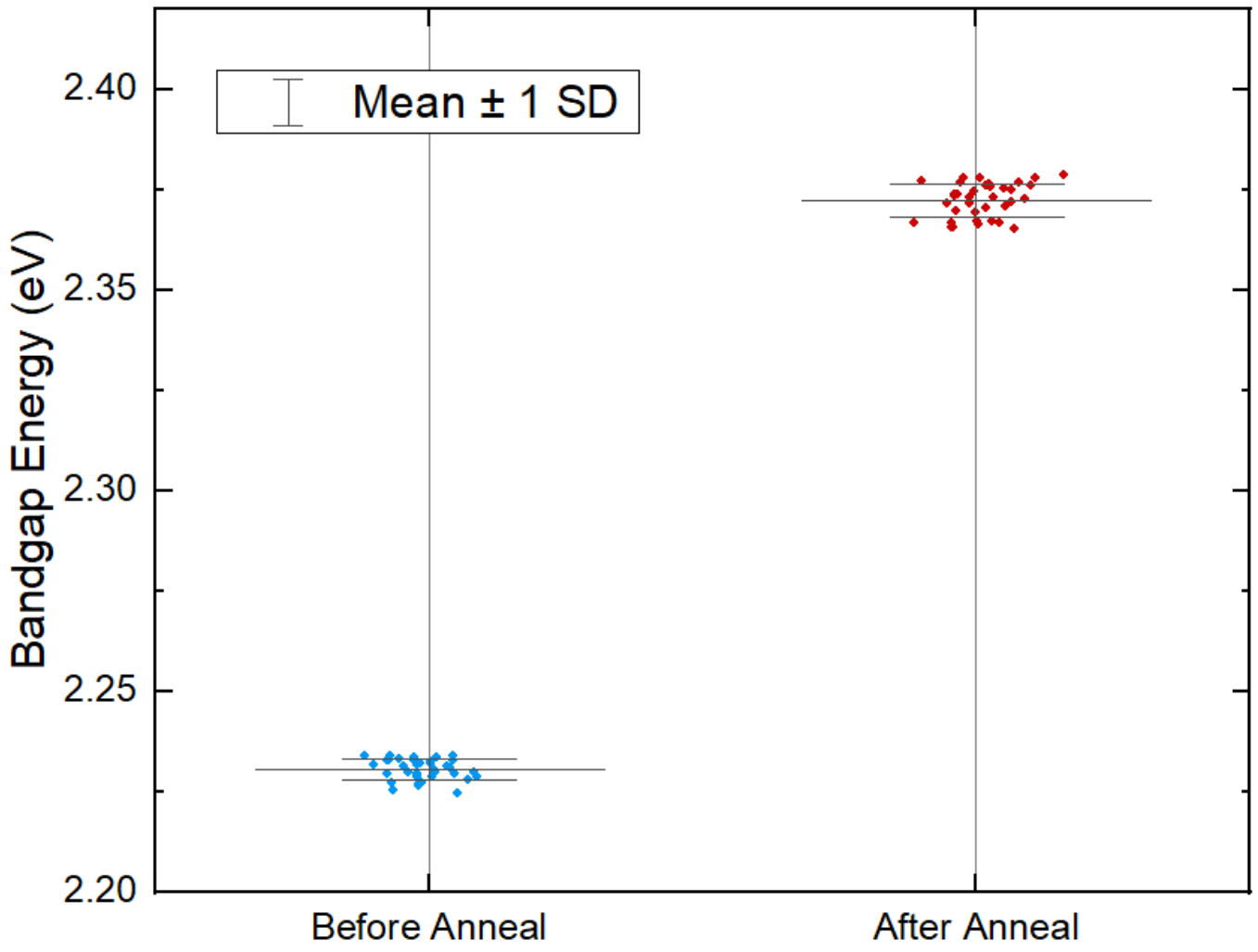
Before Anneal



After Anneal



Bandgap Distribution Statistics



Before Anneal

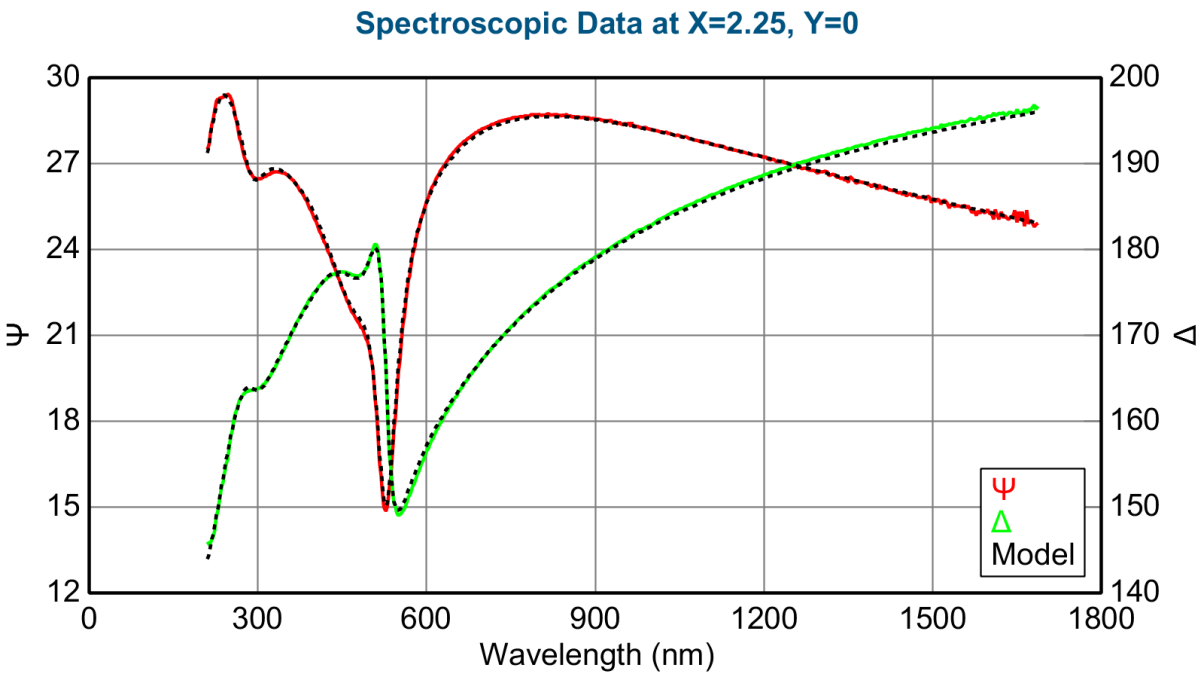
Statistic	Value
Average	2.2304
Std. Dev.	0.0026
Minimum	2.2244
Maximum	2.2339
Range	0.0095
# of Points	36

After Anneal

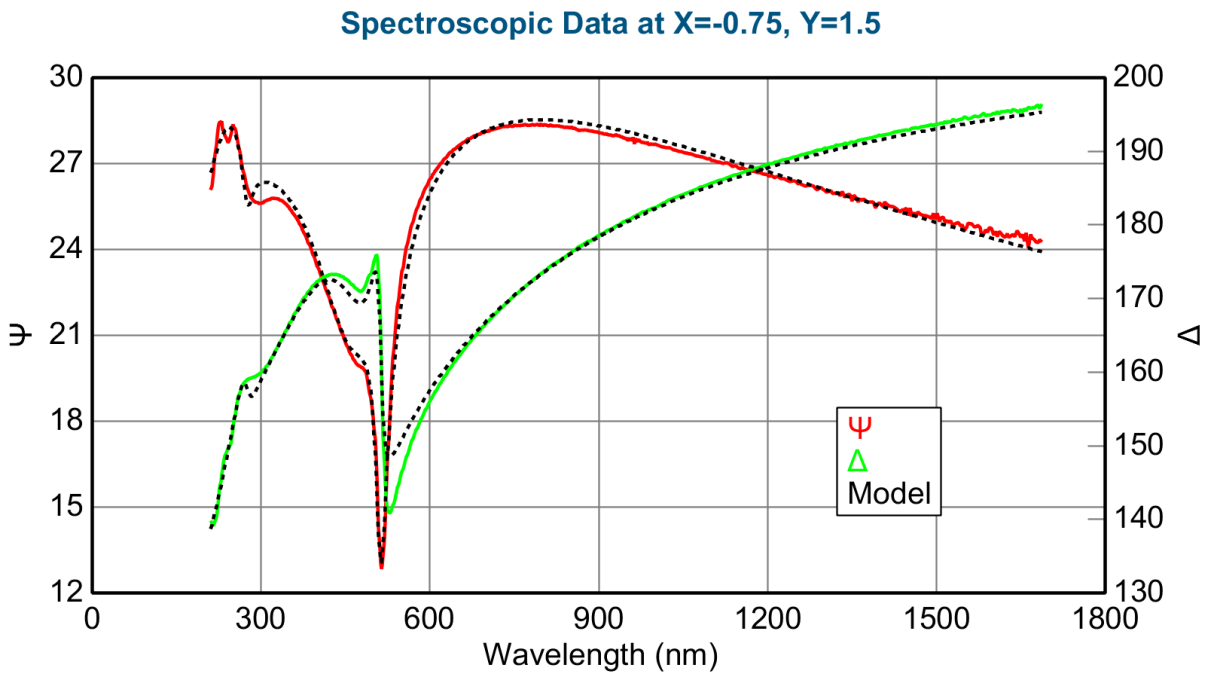
Statistic	Value
Average	2.3724
Std. Dev.	0.0042
Minimum	2.3653
Maximum	2.3786
Range	0.0134
# of Points	36

Representative Model Fits

Before Anneal



After Anneal



Modeling Details

+	Layer # 2 = Roughness Roughness Thickness = **9.31 nm** (fit)
+	Layer # 1 = CdS CdS Thickness = **96.55 nm** (fit)
	Substrate = Glass

- For both the pre- and post-anneal measurements, the three-layer model shown above is fit to the measured ellipsometric spectra at each mapping location.
- The optical properties of the CdS film are freely fit at each location and are described as the sum of three Tauc-Lorentz and one Sellmeier oscillator.
- Tauc-Lorentz oscillators are typically used to describe amorphous or disordered semiconductors and feature a variable bandgap parameter which controls the photon energy where the optical absorption goes to zero – the value of this parameter is what is mapped to determine spatial bandgap variation.
- The surface roughness is described as a Bruggeman effective medium approximation consisting of a 50/50% mix of CdS material and void.

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Appendix 1

Appendix: Instrument

J. A. Woollam Co., Inc. Model RC2-DI Spectroscopic Ellipsometer

- Dual rotating compensator configuration multichannel spectroscopic ellipsometer
- Full spectrum data acquisition in:
  - Minimum: 0.3 s
  - Typical: 10 – 20s
- Automated mapping up to 300 mm substrates
- 190 to 1690 nm spectral range
- CompleteEase modeling software
- Variable angle transmission stage
- Measurement beam diameter:
  - Normal: 5 mm
  - Focused: 300 µm

The Solution Portal can be accessed from your Order Portal dashboard

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DEMO, INC.

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Order Number	Accepted Date	Samples Received	Status	
CM000023633 1 samples, 2 techniques	2022-06-24	1	Waiting for samples	Repeat
CM000023632 1 samples, 2 techniques	2022-06-24	1	Sample Received	Repeat
CM000023631 1 samples, 2 techniques	2022-06-24	1	Sample Received	Repeat
CM000021056 1 samples, 2 techniques	2022-01-25	1	Executing	Repeat
CM000020337 0 samples, 4 techniques	NA	0	Waiting for samples	Repeat
CM000020336 1 samples, 4 techniques	2022-01-03	1	Waiting for samples	Repeat

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  - Line Edge Roughness (LER): interfacial roughness
  - Area Measurement: particle and grain size analysis
  - Line Profile: thin film thickness and multilayer measurements

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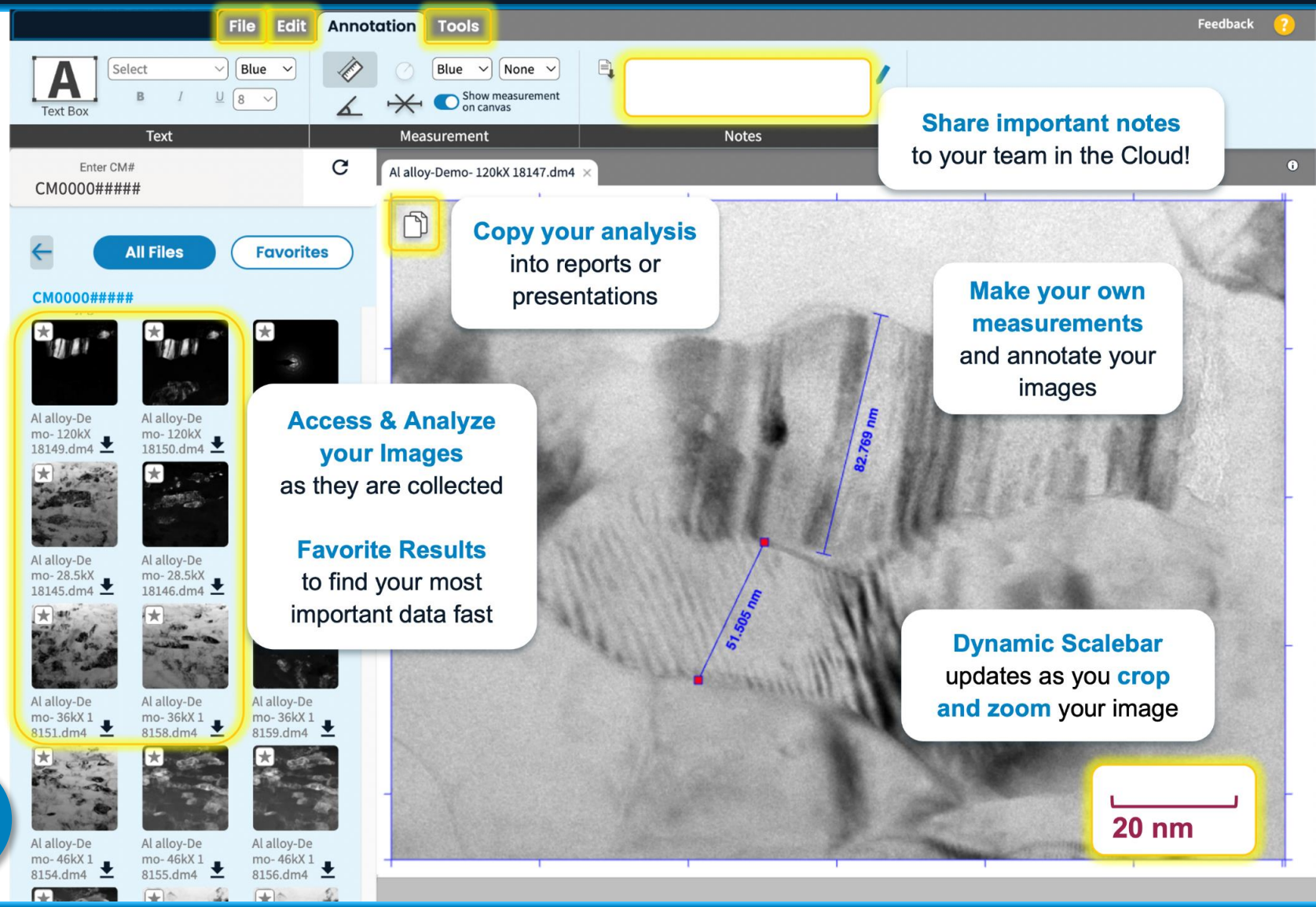

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Thank You.

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