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Spectroscopic Ellipsometry Characterization of Multi-Layer Optical Coating

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Optical coating stack performance depends on thickness and refractive index of each layer. In situ spectroscopic ellipsometry (SE) can track the layer deposition in real-time, but ex situ SE characterization is limited by the large number of unknown sample properties. Using 37-layer high-low stacks of Ta_2O_5 and SiO_2 we review various fitting methods for multilayer structures and compare their merits and limitations. One such strategy leads to a tooling parameter for each coating in the process, which can inform how the layer thicknesses of each material compare to their nominal specifications. Other strategies include tests for sources of error that can occur during multi-layer processing. Tests are shown for process drift, which would produce a gradual change in the film properties as the process continues say a slight increase or decrease in the thickness of a film or its optical constants. Another source of error that we have encountered is user-error incorrect parameter entry produces an unintentional stack design. For this case, a second multi-layer stack was deposited with an intentional thickness error for one layer in the stack. A systematic test for single-layer errors of this type easily resolved which layer in the stack had been altered.

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J.A. Woollam Co., Inc.

Ellipsometry Solutions

Spectroscopic Ellipsometry for Characterization of Multi-Layer Optical Coatings

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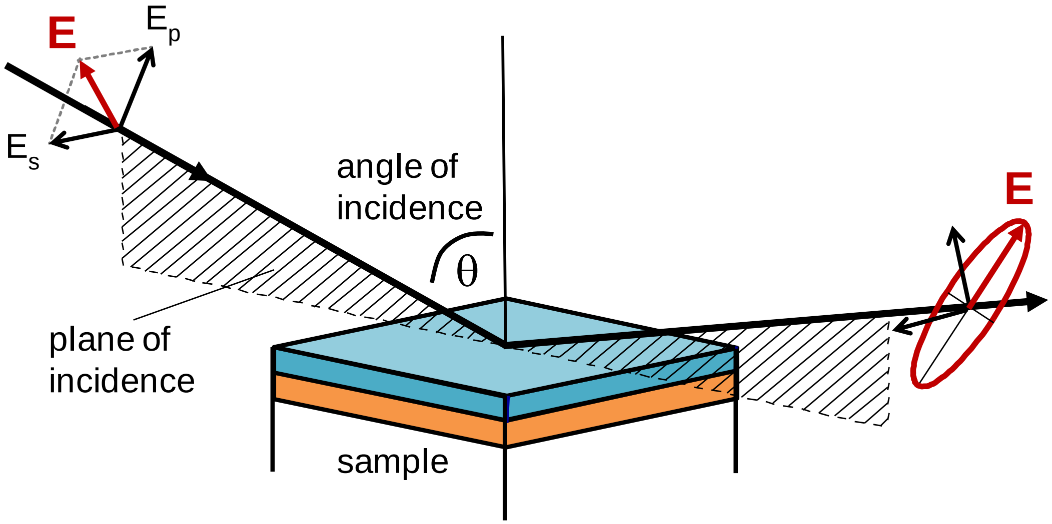
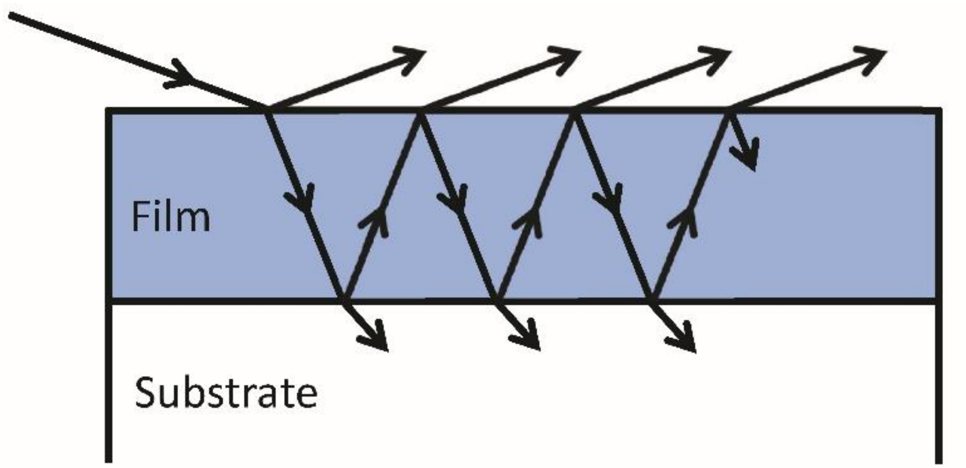
SVC 2018, Orlando, FL

Spectroscopic Ellipsometry (SE)

- SE measures polarization change as light interacts with a coated surface.



$$\rho = \tan(\Psi)e^{i\Delta} = \frac{\tilde{E}_p^{out} / \tilde{E}_p^{in}}{\tilde{E}_s^{out} / \tilde{E}_s^{in}}$$



- Coherent interference occurs when light recombines after traveling different paths through thin film.

Data Analysis

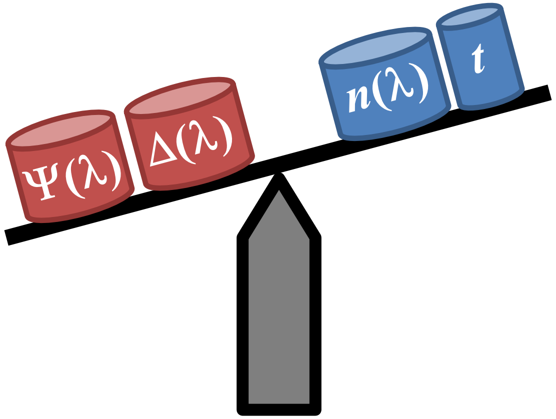
Measurement Information

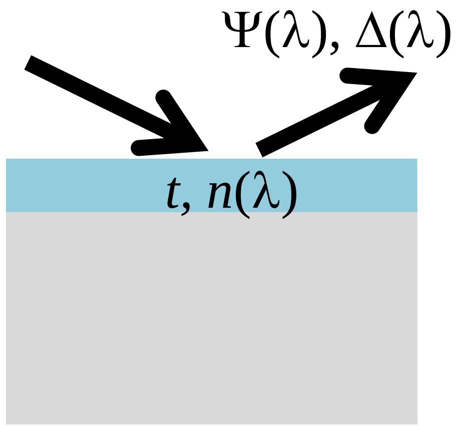
- Total content is **<u>2λ</u>**.
- Multiple angles may add extra information.

Sample Properties

- Film thickness
- Optical Constants
  - Transparent (*n*): **<u>1λ</u>**
  - Absorbing (*n* & *k*): **<u>2λ</u>**

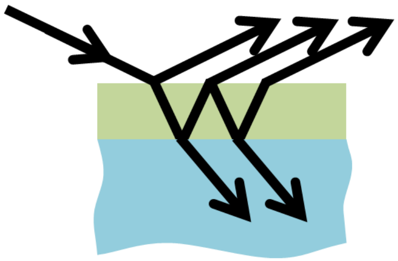
- Need data content to determine all unknown sample properties

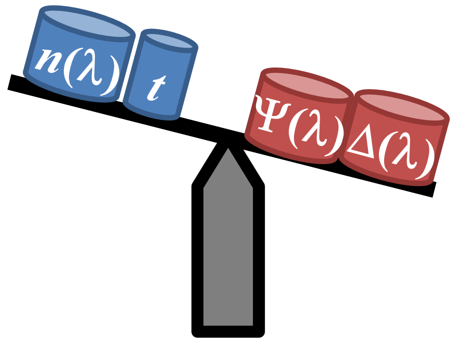


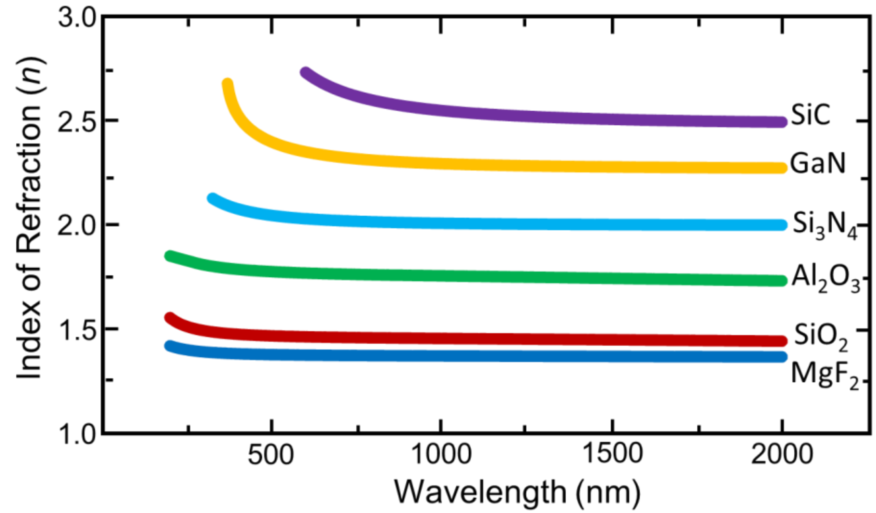


Transparent Film (thickness and *n*)

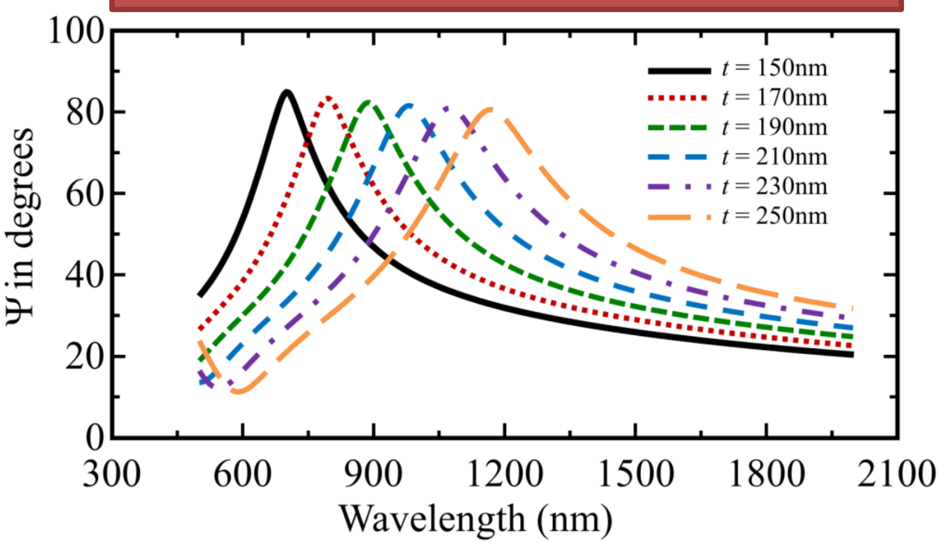
- Most common SE application
  - Use dispersion equations



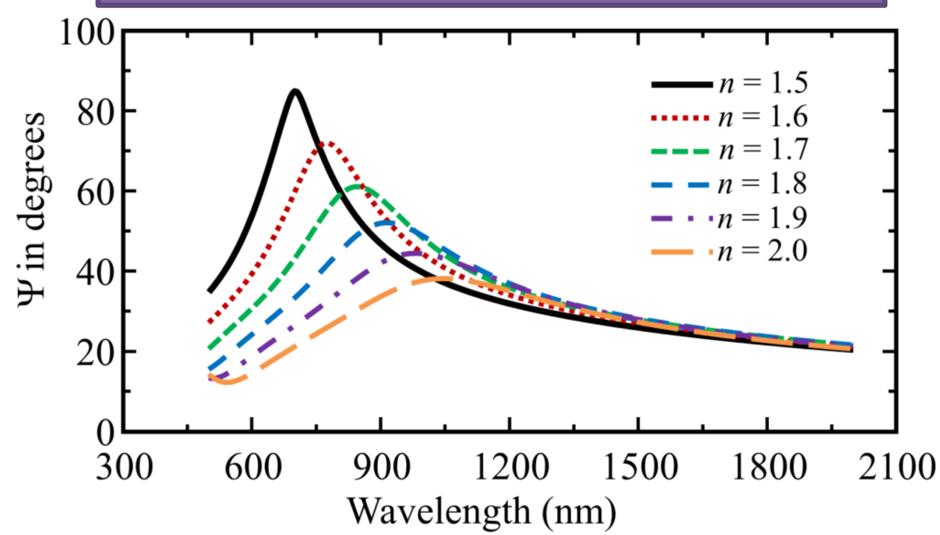




Thickness shifts interference

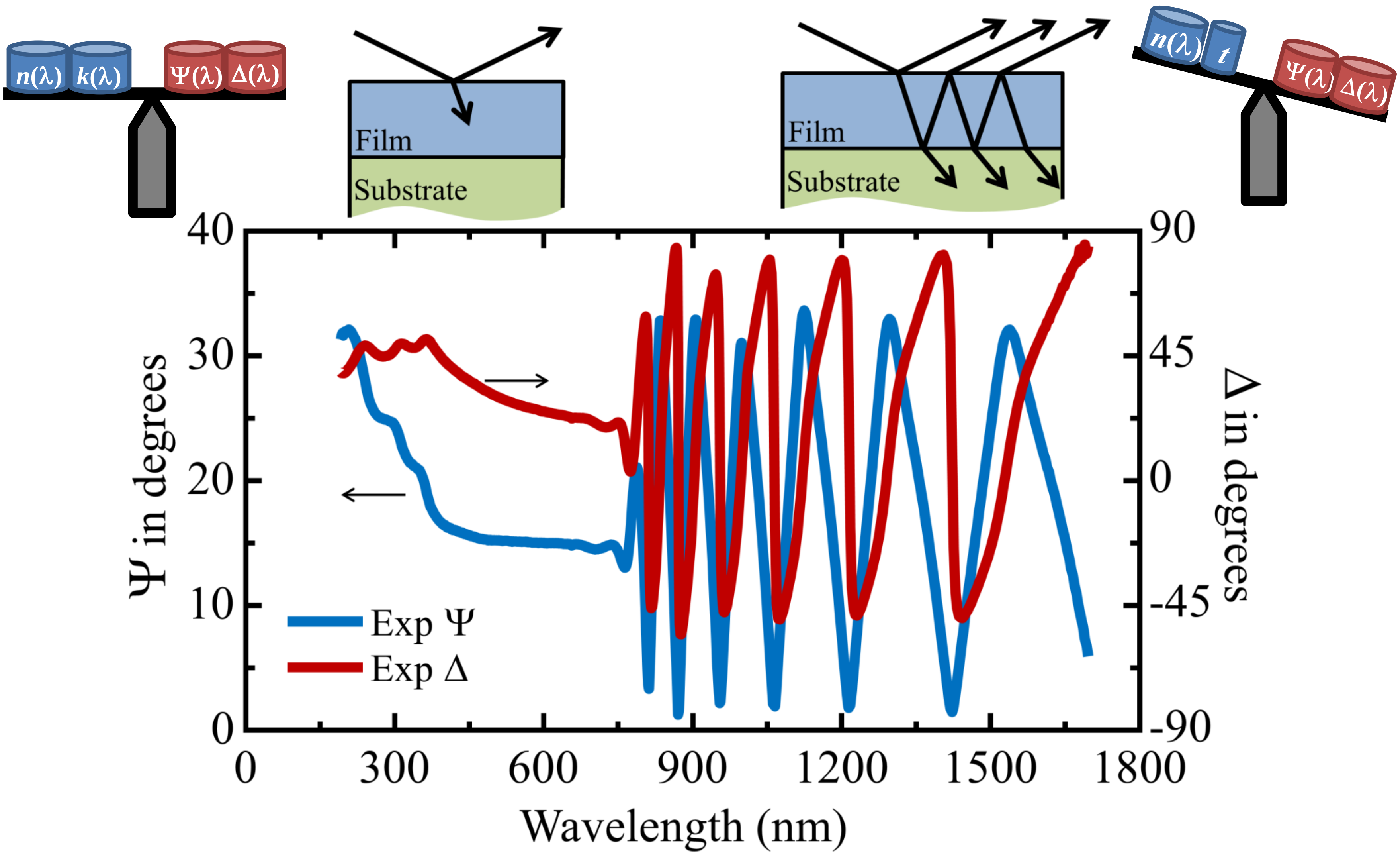


Index also affects amplitude



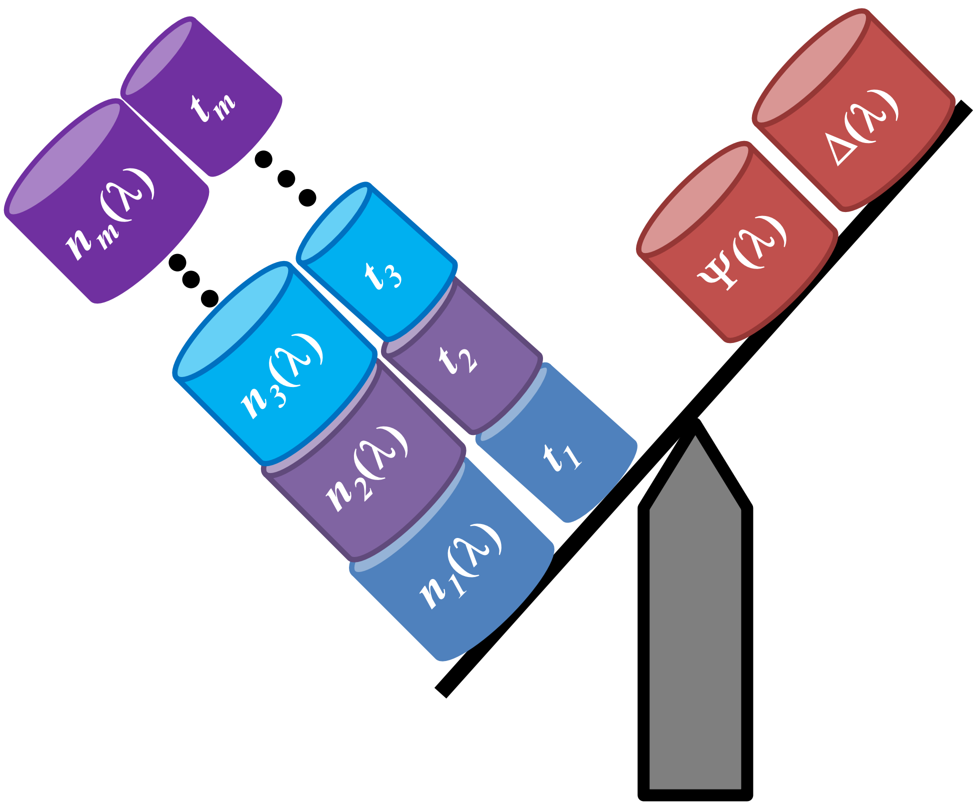
Films with absorbing spectral regions

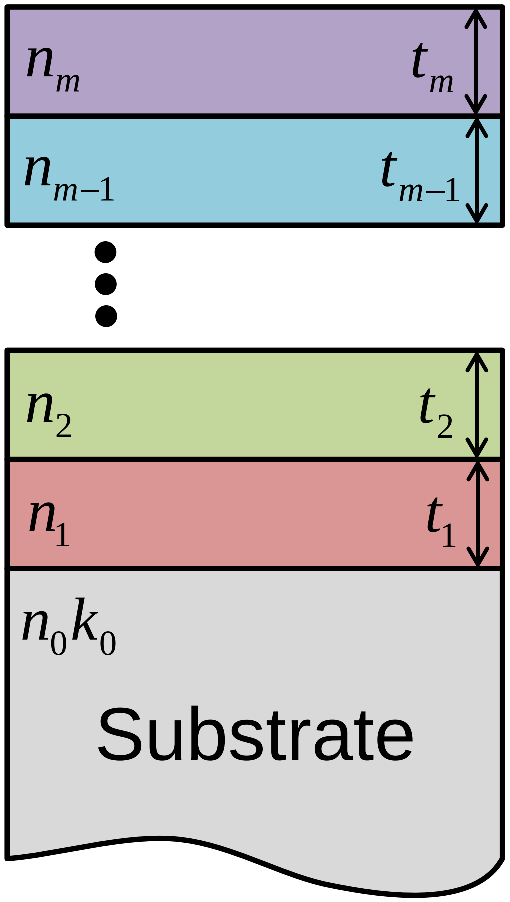
- Spectroscopic data determines thickness, *n* and *k*.



Multilayer Stack Challenge

- Multilayer applications have an excessive number of unknowns.





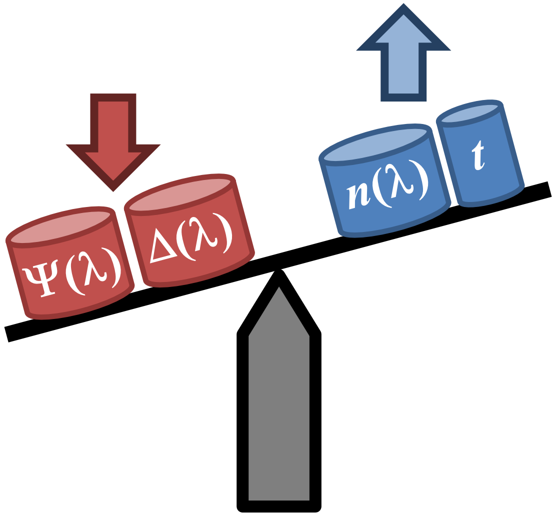
Ellipsometry Strategies

Increase Measurement Content

- Wide Spectral Range
- Multi-Angle
- Multi-Sample
- In-Situ (Real-Time)
- SE + Transmission

Reduce Sample Unknowns

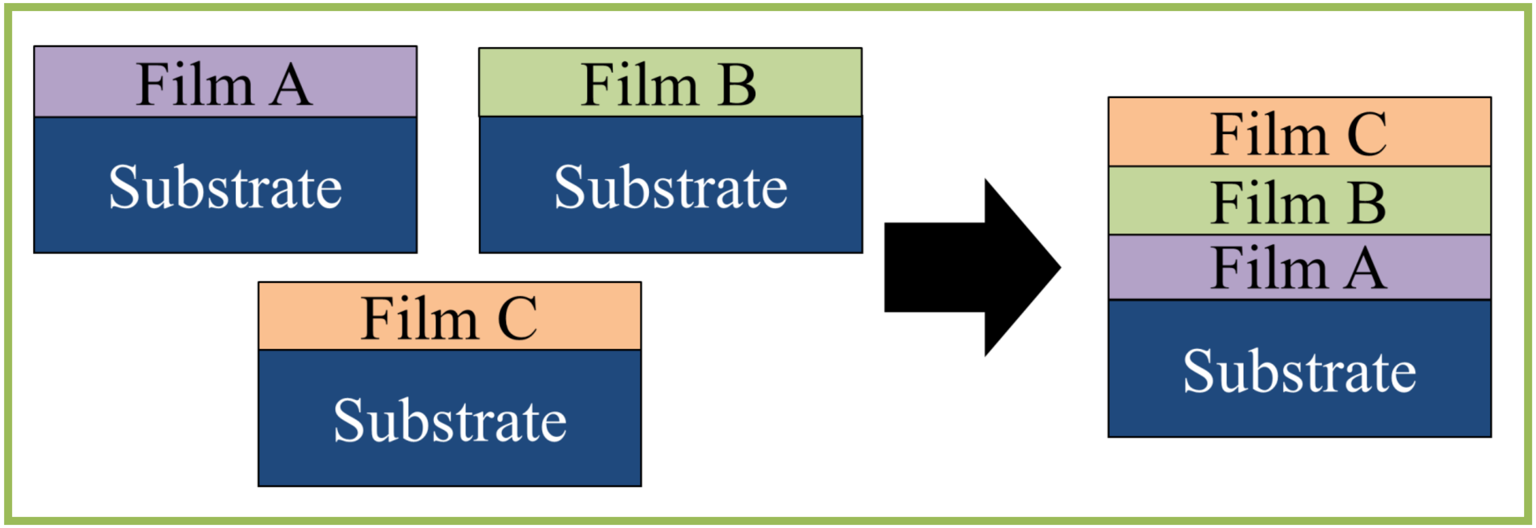
- Opaque Wavelengths
- Transparent Wavelengths
- Fixed *n*,*k*
- Coupled *n*,*k*
- Fixed Thicknesses
- Coupled Thicknesses
  - Superlattice
  - Tooling Factor (ratios)

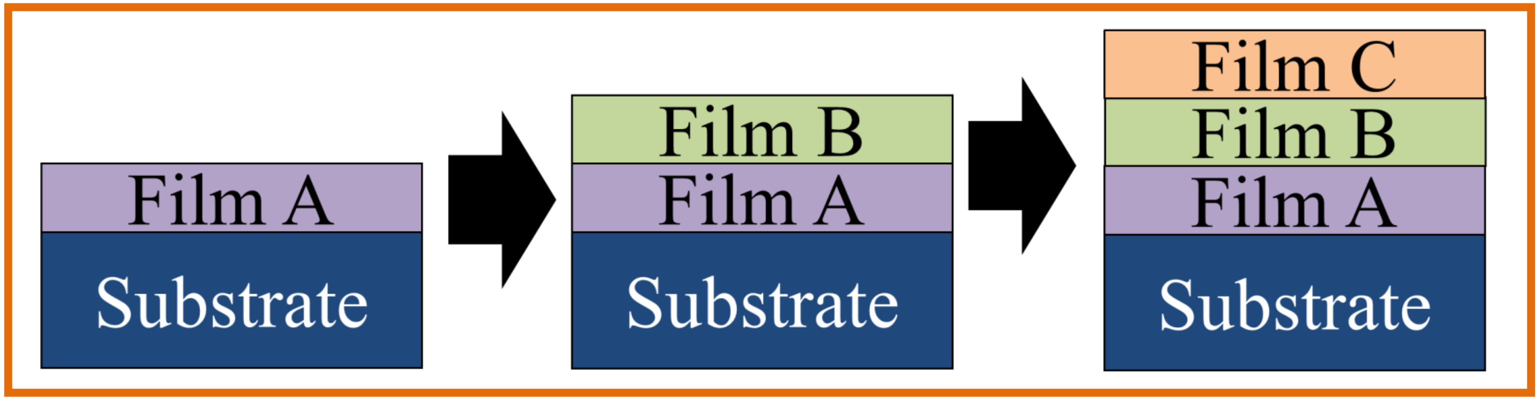


J. Hilfiker et al. *Thin Solid Films* **516** (2008) 7979-7989

Multilayer Strategies

- Determine optical constants from single layers.

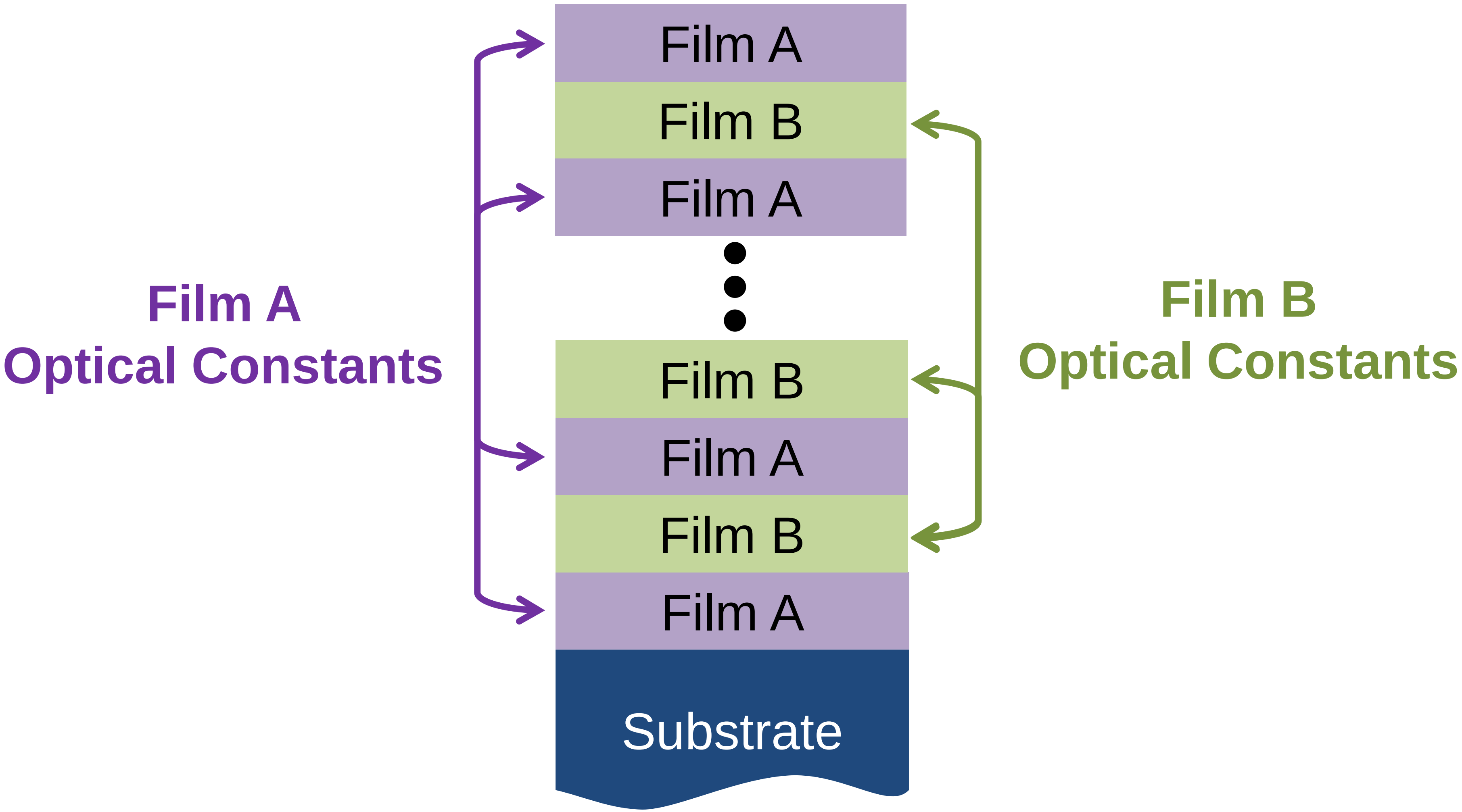




same unknowns as 1-layer

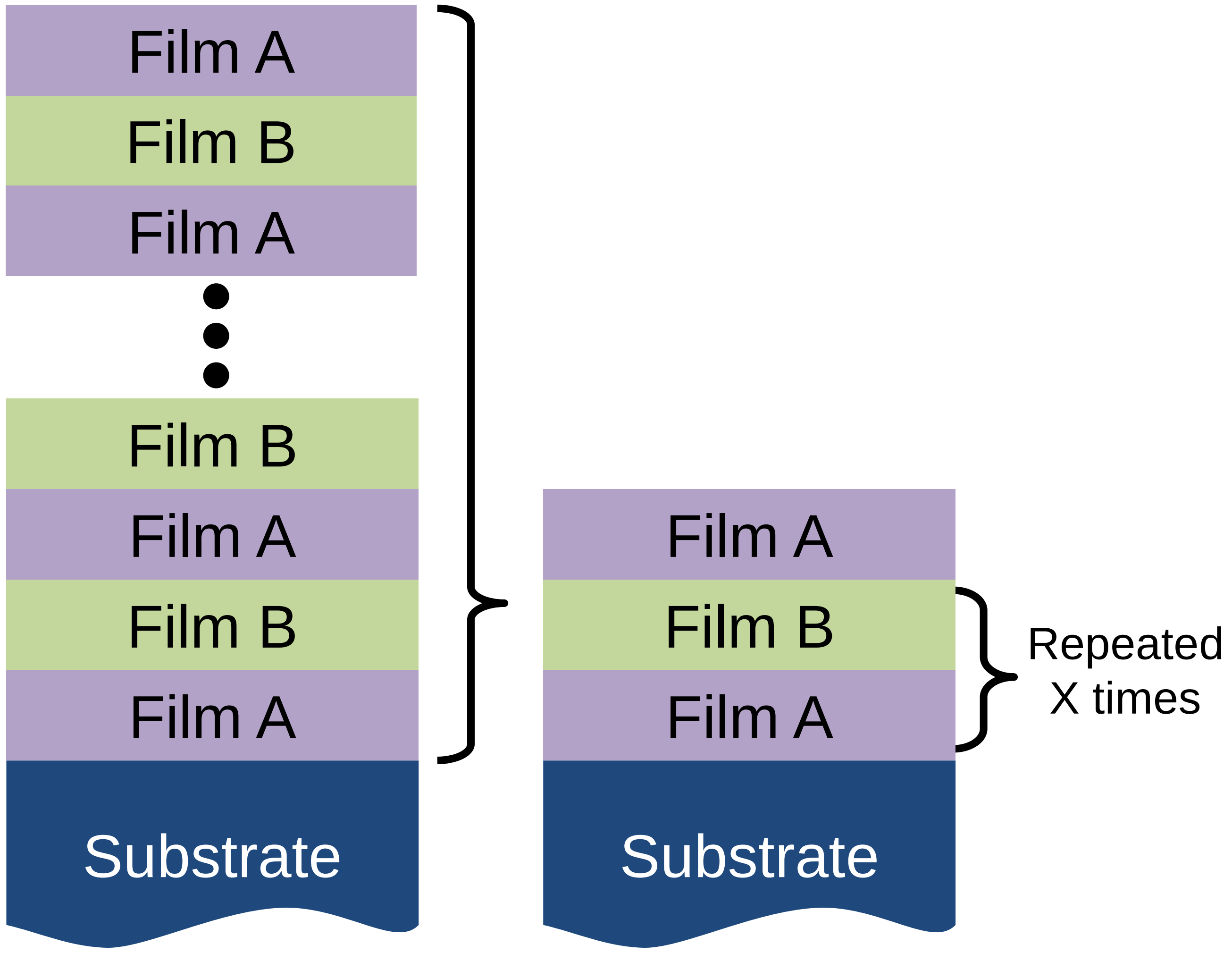
Multi-Layer Strategies - 2

- Couple optical constants for same materials.



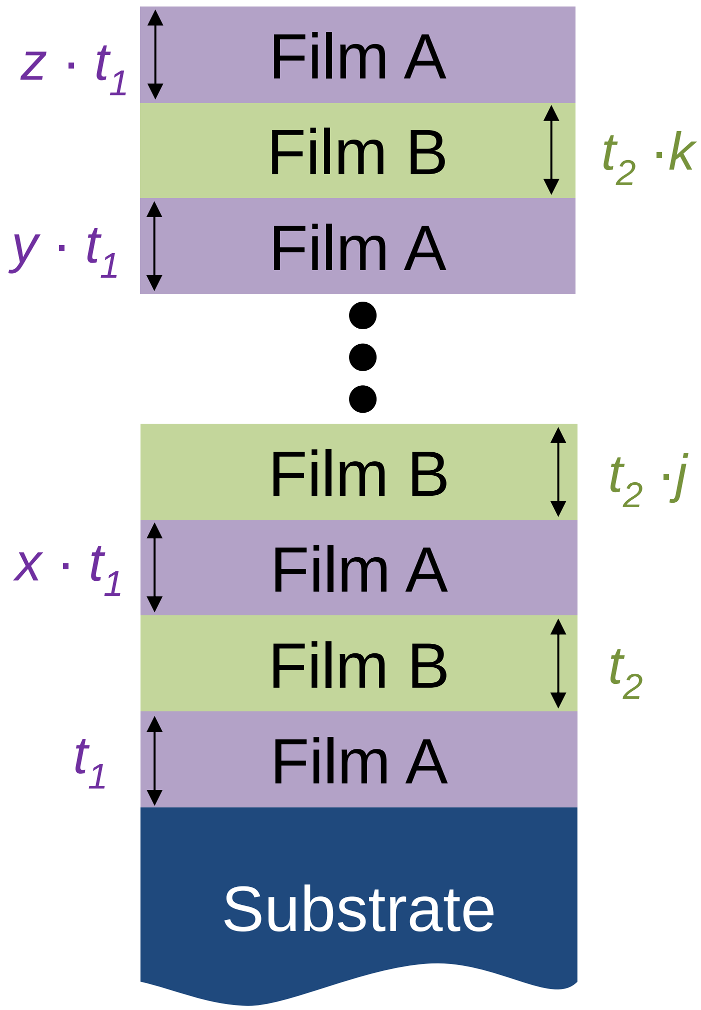
Multi-Layer Strategies - 3

- Couple "like" thicknesses <u>and</u> optical constants



Multi-Layer Strategies - 4

- Create "Tooling Factors" to maintain thickness ratios.



37-Layer Optical Coating Stack

- Near infrared optical coating design sputter deposited using high index (Ta_2O_5) and low index (SiO_2) layers

- Samples:
  - Single-layers of each coating
  - 4-Layer Stacks
  - 37-Layer Final Design
  - 37-Layer “Blind Test” – 1 discrepant layer

- Spectroscopic Ellipsometry
  - Wavelengths: 190nm to 1700nm, with 750 individual points
  - Angles of Incidence: 45°, 55°, 65°, and 75°

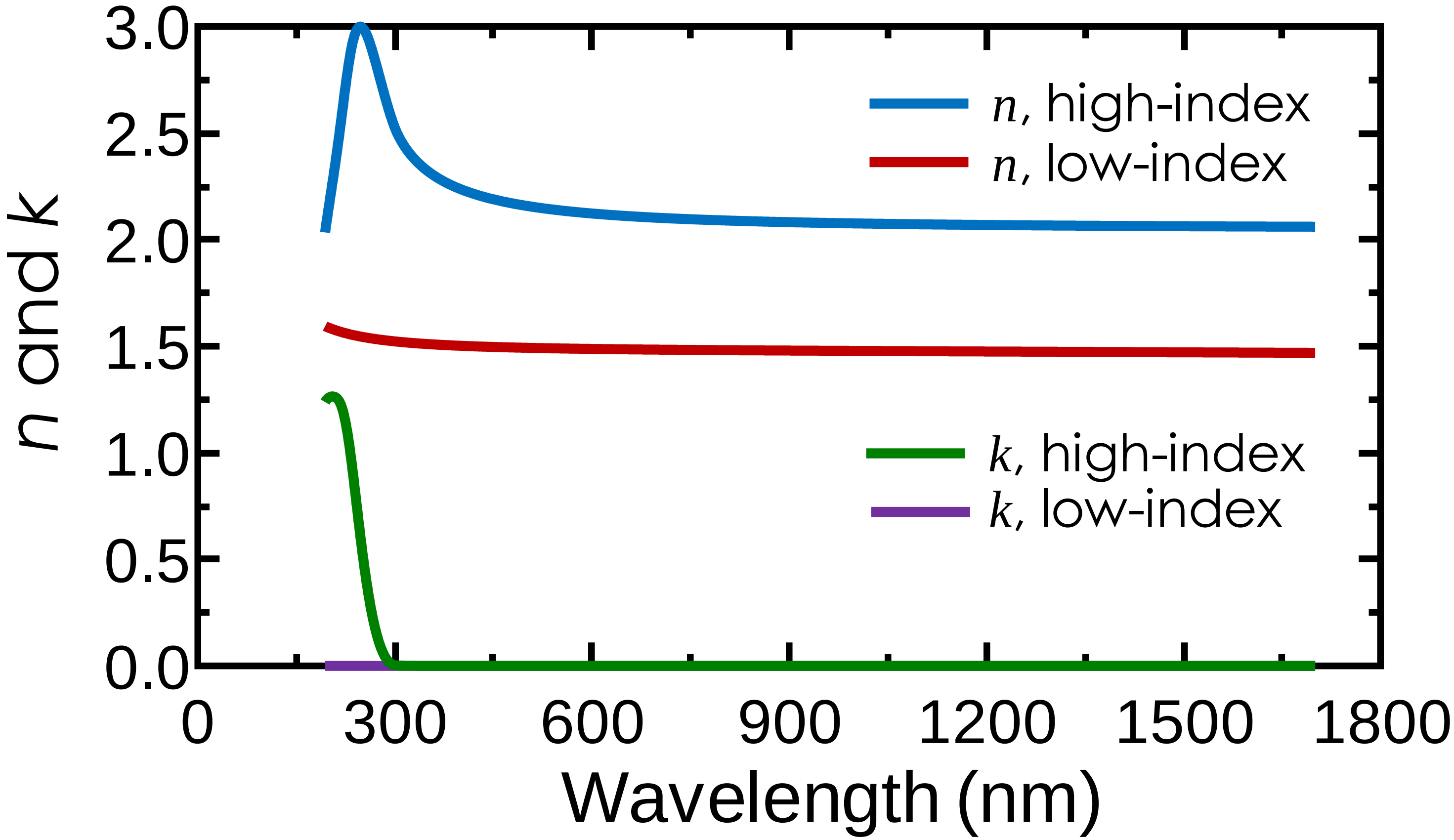
Single-Layer Coatings

Low-Index

- Sellmeier dispersion equation
  - 3 fit parameters

High-Index

- Sum of oscillators
  - 11 fit parameters



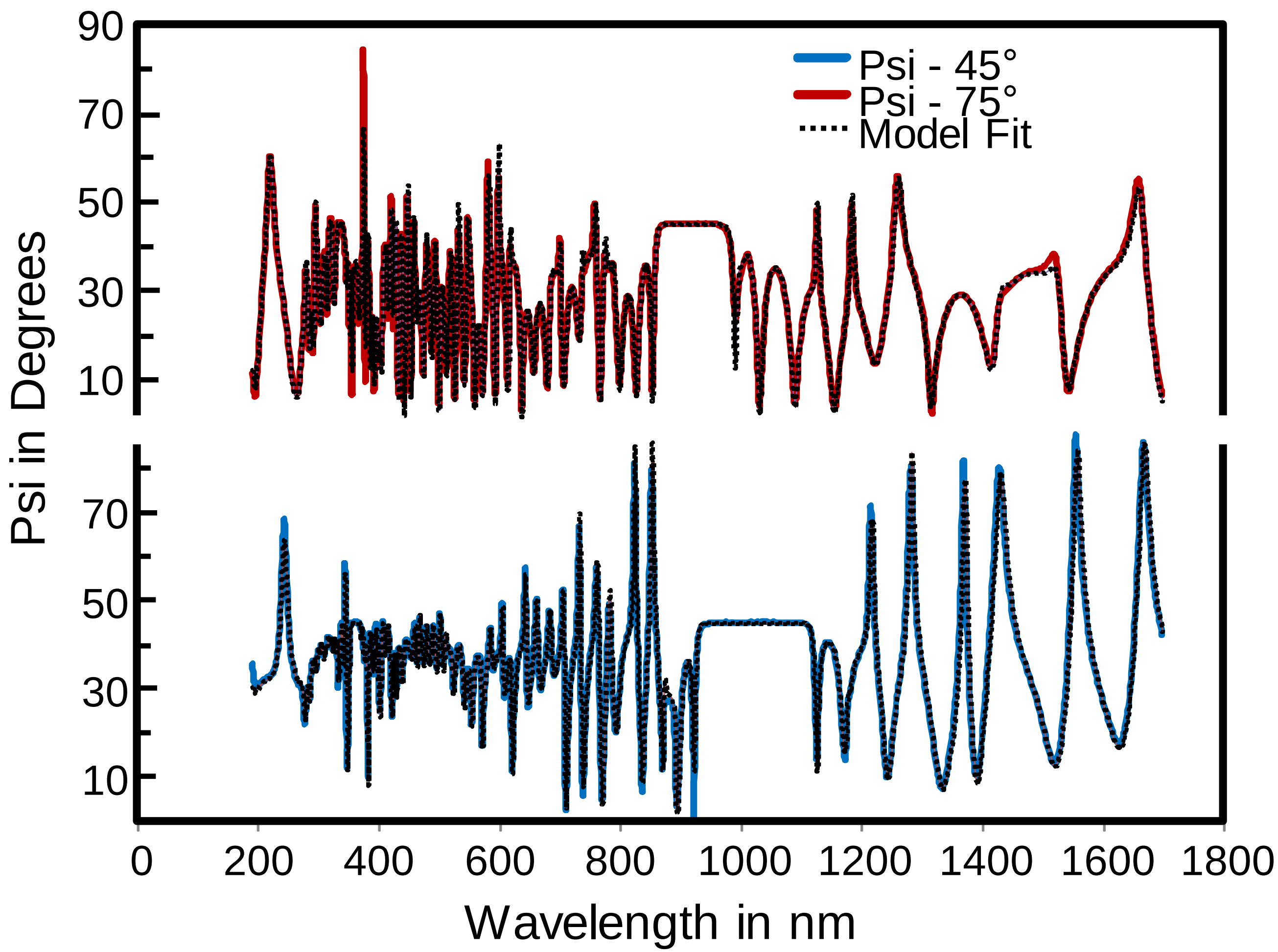
37 Layer Stack Analysis Tests

- Optical Constants:
  1. Fixed from single-layers
  2. Fixed from 4-layer stack
  3. Float dispersion equations for Low-*n* and High-*n* (coupled)
- Thicknesses:
  - Establish "Tooling Factors" for Low-*n* and High-*n*
  - Add Linear Variation to each "Tooling Factor"
  - Fit Individual Layers
  - Fit All Layers

Layer No.	Design Thickness (kÅ)	Material	RATIO1	RATIO2
1	1.813	Low-n	1	
2	1.262	High-n		1
3	2.216	Low-n	1.22	
4	1.255	High-n		0.99
5	2.102	Low-n	1.16	
6	1.336	High-n		1.06
7	2.094	Low-n	1.15	
⋮				
29	2.218	Low-n	1.22	
30	1.048	High-n		0.83
31	2.221	Low-n	1.23	
32	1.326	High-n		1.05
33	2.224	Low-n	1.23	
34	1.053	High-n		0.83
35	2.217	Low-n	1.22	
36	1.119	High-n		0.89
37	2.222	Low-n	1.23	

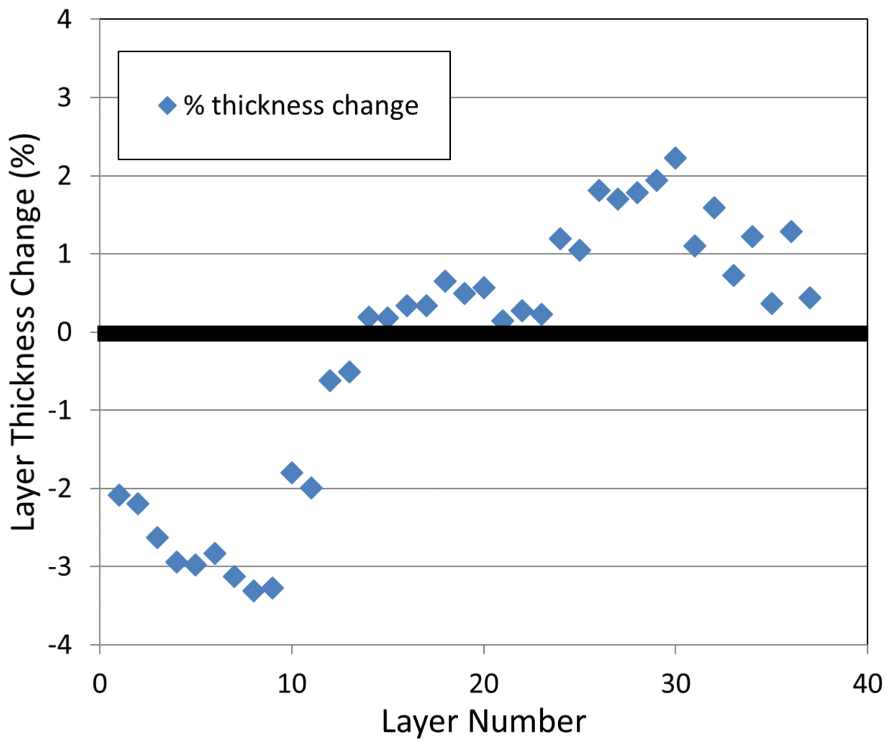
37-Layer Stack Data Fits

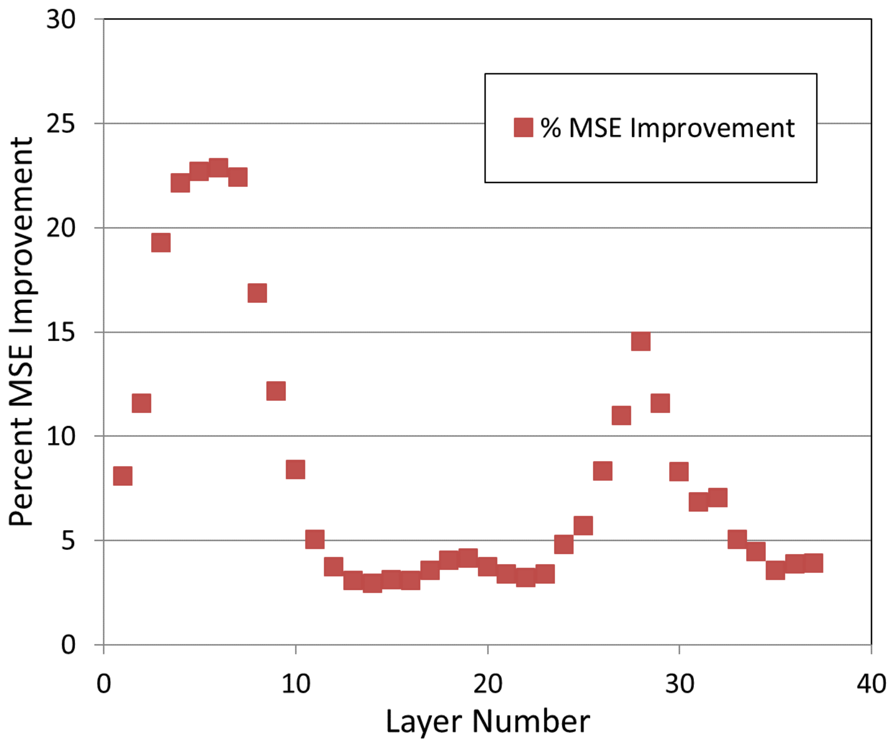
- Quick match to the data is found by fitting optical constant dispersion and 2 tooling factors: Ta_2O_5 (100.4%) and SiO_2 (97.4%)



Testing Individual Layers

- Systematically allow 1-layer thickness to be free from the tooling factors during fitting.

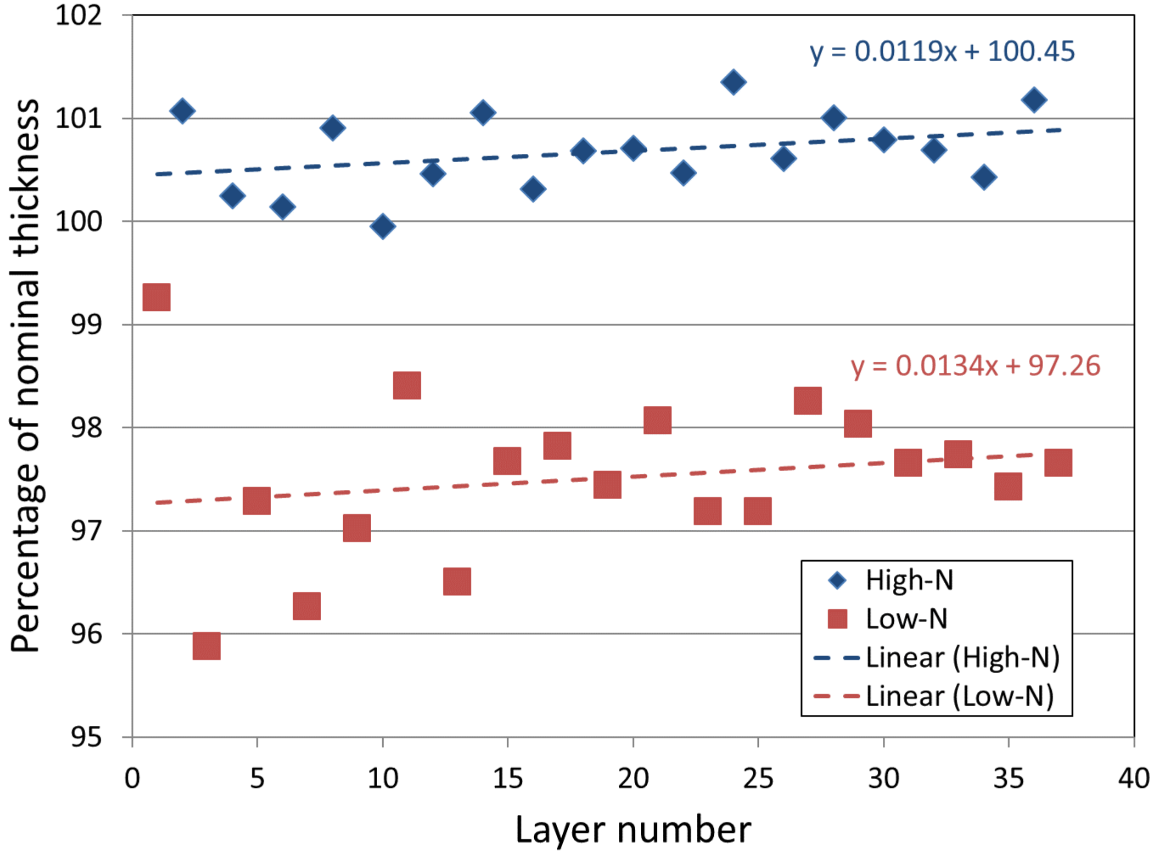




$$MSE \propto \sqrt{\sum (Model - Experiment)^2}$$

Fitting All 37 Layer Thicknesses

- View noise-limit when fitting large # of parameters.
- Layer thicknesses are near fit results using Tooling Factor with a slight linear increase.

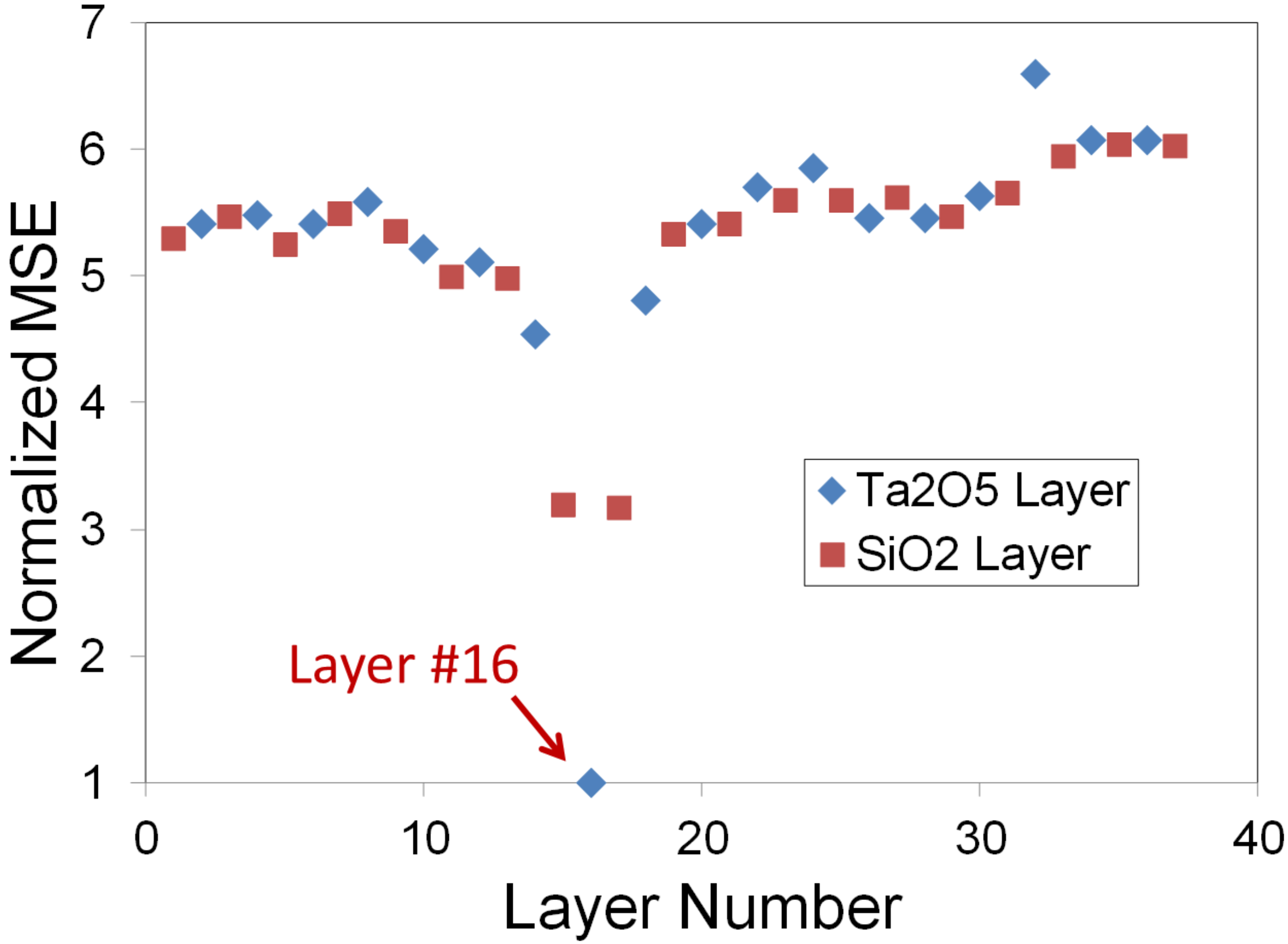


Comparison and Results

Model #	Optical Constants	Ta_2O_5 Thickness	SiO_2 Thickness	# Fit Parms	MSE
1	*n,k* from single-layer	102.20%	97.60%	2	115
2	fit *n,k* for each material	100.40%	97.40%	17	80
3		4 Tooling Factors Layers 30-37: 100.76% Layers 20-29: 100.69% Layers 10-19: 100.52% Layers 1-9: 100.29%	4 Tooling Factors Layers 30-37: 97.56% Layers 20-29: 97.79% Layers 10-19: 97.55% Layers 1-9: 97.07%	23	57
4		Tooling Factor + Slope 100.26% Slope = +0.025%	Tooling Factor + Slope 97.22%, Slope = +0.013%	19	60
5		All layers fit	All layers fit	52	48

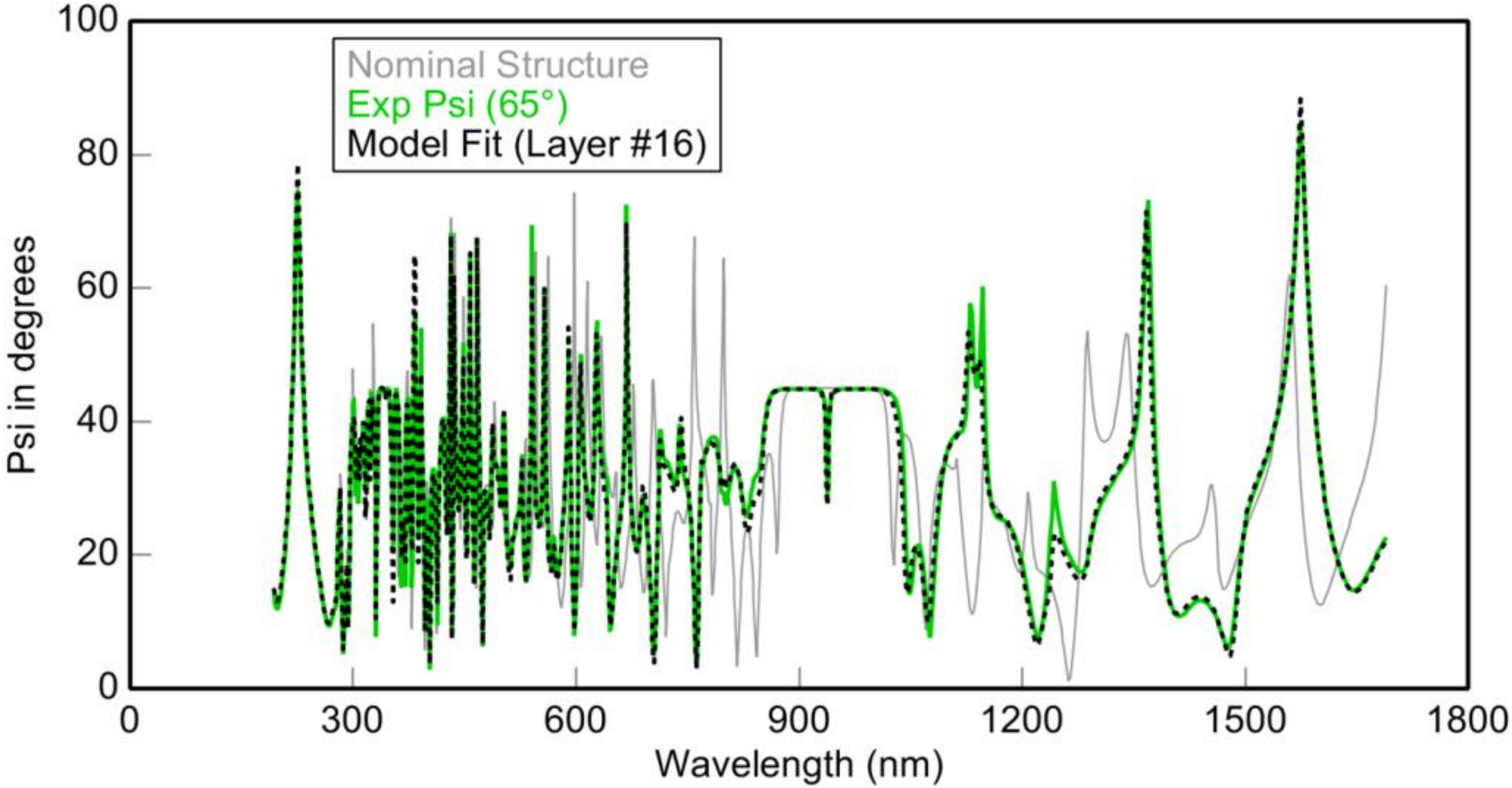
Blind Test: Error in 1 layer

- 1 layer intentionally modified to study whether SE can identify location of discrepant film?



Blind Test: Error in 1 layer

- Layer #16 (Ta_2O_5) is clearly incorrect (verified after analysis), with a resulting layer thickness of double the nominal value.



Conclusions

- Multilayer structures can be measured with SE, but may require special methods to either:
    - Reduce unknown sample properties.
    - Increase measurement information content.
- Single-layer films help determine optical constants and dispersion equation parameters.
- Optical Constant coupling significantly reduces the total number of unknowns – for repeated materials.
- Thickness coupling reduces total unknowns. A “Tooling Factor” enforces known thickness ratios between layers to vary thickness of similar films by the same percentage.
- Some process variations can be identified due to high sensitivity of SE to the data dispersion.