

Computer Techniques for Improving Optical Coating Yields

Main Points and Comments

Fred Goldstein FTG Software Princeton, New Jersey

1. Material Properties

Really important

Use design software to generate *Gedanken Spectra* for determining the conditions where it is possible to deduce n, k for your combination of film thickness and measurement apparatus, etc. Add noise to generated spectra to predict expected accuracy.

Envelope method

A thick layer of a material with $k \ll n$ ($k \sim 0$ and n non-dispersive at maximum wavelength) is measured in transmittance (or reflectance). At long wavelengths, peak (even quarter waves for T) and valley (odd quarter waves) positions are proportional to the ratio of whole integers and the index of refraction n is simply related to the peak-valley amplitude difference.

This *preliminary* method is simple and accurate for well-behaved films, but inaccurate for absorbing films.

Parametric fit method

Assumes that n, k vs. wavelength can be described by continuous functions (*Determination of Optical Constants.pdf*). Useful functions include Lorentzian and generalized Cauchy. (WN is wavelength in nm, WM is wavelength in μm .)

$$\begin{aligned} \text{Lorentzian: } x_1 &= \text{WN}^2 - C^2, \quad x_2 = x_1^2 + D^2 * \text{WN}^2 \\ n &= \text{Sqr}(A + k^2 + B * \text{WN}^2 * x_1 / x_2), \quad k = (.5 / n) * B * D * \text{WN}^3 / x_2 \\ \text{TiO}_2\text{A: } A &= 4.71, \quad B = 0.215, \quad C = 390.2, \quad D = 0.447 \end{aligned}$$

$$\begin{aligned} \text{Generalized Cauchy: } n &= A + B * \text{WM}^D + C * \text{WM}^E, \quad k = \text{Exp}(F + G * \text{WM}^H) \\ \text{TiO}_2\text{A: } A &= 9.4896, \quad B = -7.3169, \quad C = 5.081\text{E-}3, \quad D = 6.18\text{E-}3 \\ E &= -4.4077, \quad F = -9.8247, \quad G = 5.064\text{E-}2, \quad H = -4.9717 \end{aligned}$$

Step-by-step procedure with *FilmStar DESIGN* steps italicized:

- Measure %T and/or %R at normal and/or non-zero angle (polarizer needed).
- Import spectra, convert to optimization targets (*Optimize..Targets..Setup..Generate*).
- Assign dispersive index function from a similar material. Lorentzian (4 coefficients) and generalized Cauchy (8 coefficients) should work for most oxides. (*Setup..Film Indices..Insert Function*).
- Interactively (*Evaluate..Interactor*) determine a reasonable starting guess for film thickness (in physical thickness, do not use optical thickness here).
- Select layer thickness and film index as variables (*Optimize..Variables*). It should not be necessary to assign limits to index coefficients.
- Solve for thickness and indices via DLS refinement (*Optimize..Optimize*).
- Verify results by comparing calculated and measured spectra. Copy index function to clipboard (*Setup..Film Indices..Edit..Copy Function*) and paste into INDEX (*INDEX: Functions..Fit Index..Edit..Paste Function*). Compare graphically with initial function. Does it look reasonable?

Point-by-point method

BAD NEWS: a half wave of a non-absorbing material *disappears*! GOOD NEWS: at the same wavelength, the film is not a half wave at a non-zero angle. This indicates the importance of non-normal incidence measurements!

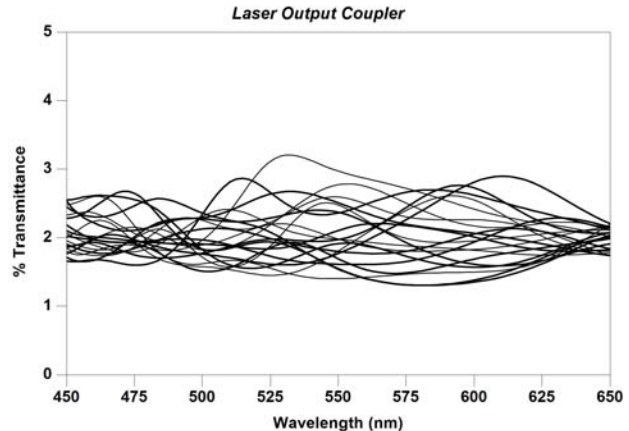
2. Estimating Yields

Tolerancing

Monte Carlo methods are widely utilized for estimating yields and comparing different coating designs. Both thickness and index variations can be included.

Results are typically represented graphically, but this might not be sufficient as it is difficult to deduce yields.

Spreadsheets provide a method for calculating yields for the most complex specifications.



3. Reverse Engineering

Free version

For attendees who do not have the latest version of FilmStar DESIGN, examples in this section work with the Free Version available at <http://ftgsoftware.com/fsfree.htm>.

Gross errors

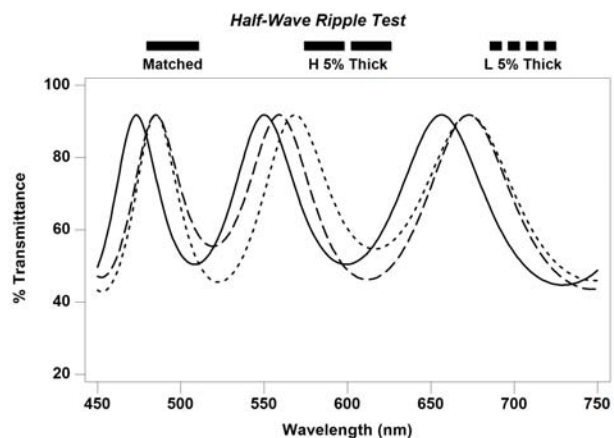
Refinement methods do not work when layers are missing from (or added to) the design! Coating operators may fall asleep, visit the toilet, eat snacks, etc. Automatic controllers might restart a layer after a glitch, etc. Interactive inspection is critical!

Inverse-synthesis

In inverse-synthesis, measured spectra are converted to optimization targets and thickness and/or index deviations are deduced by starting with the ideal layer stack and 'designing' the measured spectrum.

There is great simplification if errors depend only on tooling factor changes. Here material ratios are treated as optimization variables. The well-known (?) *Half-Wave Ripple Test* uniquely identifies imbalances.

More generally we must that all layers vary. Is the solution unique? A method for deducing the reliability of inverse-synthesis is introduced (*In FilmStar DESIGN use FilmSolve*.bas*):



- Starting with ideal *Design A*, randomize layers and obtain modified *Design B* which simulates manufacturing errors.
- Calculate the *Design B* spectrum and convert to optimization targets. Targets at multiple angles and polarization may be added.
- Restoring *Design A*, deduce layer changes by least-squares optimization; all layers are varied. The resulting layer stack is *Design C*. Ideally *Design B* = *Design C*. Let's say that inverse-synthesis is reliable if all *Design C* layers are within 0.5% of (known) *Design B*.
- The above steps are repeated many times until the statistics become clear.

To the best of this author's knowledge, this procedure has not been published. In tests with our 26 layer Laser Output Coupler design (measured in %T up to 1200 nm), reliability ranges from zero (0° only) to 100% (0° plus 45° S and P pol).

Question: is there a global minimum?

Correction functions

Assuming reliable inverse synthesis, layer errors will be random or systematic. Systematic errors may depend on layer thickness (*i.e.* crystal monitor with non-ideal relation between physical and optical thickness) or total thickness (*i.e.* tooling factor shifts caused by material depletion).

Deviation plots indicate whether errors can be correlated to layer or total thickness. Correction functions can be deduced by least-square fitting and functions such as

```
Function CF_L!(Byval qLay!) ' qLay is Layer Thickness (QWOT=.25)
    CF_L = 1.00307 - 3.9517E-2 * qLay
End Function
```

utilized to adjust monitor thickness.

4. Optical Monitoring

Why monitoring software?

Since design software predicts all optical properties, why is there need for a separate program to translate designs to optical monitor recipes? Consider the following procedures for turning 'monitoring curves' (R/T vs. thickness) into machine settings:

- a) Each witness chip has its own thin film design. Try 2 to 4 layers on a chip. In the case of a Leybold 6 or 12-position witness, too many layers on a spot will result in monitoring errors; this configuration requires an easy way to change layer assignment.
- b) Multiply each sub-design by monitor-to-work (tooling) ratio and evaluate over a range of wavelengths to determine optimum cutoffs. Include index variations between design and monitor, system spectral response, and monochromator calibration. The latter is critical when a wide range of monitor wavelengths is required.
- c) Calculations should utilize the last two turning points. These may be in previous layers when monitoring thin layers (use the same wavelengths for all layers on a chip).
- d) If it's not possible to find good cutoff ratios, change the number of layers on the chip.
- e) Recalculate to ensure the monitor signals stay within appropriate levels for manual or automatic monitors. You don't want to go off-scale during the run.
- f) Manual monitors - Create a run-sheet with coating instructions, including starting level for each chip. Embedding strip-chart plots in the run-sheet helps technicians 'get it right'.
- g) Automatic monitors - Print monitor settings for typing data into older systems (Balzers GSM-420), upload settings via RS-232 (Eddy LMC-20) or create a coating file (Leybold Leycom IV, SYRUSpro) as appropriate.

Direct and indirect monitoring

Generally, there are two types of optical monitors: direct and indirect. In direct monitoring, the actual part is monitored, usually for quarter-wave designs such as narrow band filters. Layers are inaccurately terminated at quarter-wave peaks and valleys, but compensation effects result in highly accurate results.

In indirect monitoring (witness chips) there is no compensation effect (some would argue about this point) but layers are terminated accurately. While most monitors operate at a single adjustable wavelength, there are monitors which measure the entire spectrum. There are monitors using a cassette of witness chips and monitors where there are re-usable witness spots.

One company's monitor recalculates optical properties and attempts to compensate for shifting indices, while another company thinks that approach is useless. There is controversy and frustration amongst users, perhaps compounded by the overly mathematical approach taken by some.

One important point is that the cut algorithm include turning points in previous layers. We point this out because it is not always implemented and is very important for thin layers.

Manual monitors

Probably most optical monitoring is manual, with a trained operator watching a strip chart and cutting layers when given ratios are achieved. In such cases coating yields are improved by ensuring that operators understand how to cut layers. An important ingredient is the ability to produce operator instructions (typically called coating run-sheets) in local languages.

Next is the Coating Game © simulator used to ensure that run-sheets are well understood. At the end, *My Coating* is compared to the original design.

Automatic monitors

Several examples are illustrated at length. No matter what model, it is our job to decide on chip distribution and monitor wavelengths. To avoid mistakes it is *important that final instructions be automatically uploaded*; no one should accept a machine where it is necessary to type values.

5. Crystal Monitoring

Advantages

Simplicity! There is no need for elaborate software to convert designs into monitor settings. Reports indicate that crystal monitors work better than ever, probably due to improvements in coating processes.

Correction functions

Secret of success? Here is where we utilize the correction functions previously discussed under *Reverse Engineering*.

Uploading layers

While typing layers is not a problem for AR coatings, it is a source of mistakes when there are many layers. One recommended procedure is to have one person type the values and another verify them. Once again, no one should accept a machine where it is necessary to type values.