'Gedankenspektrum' Methods in Optical Coatings

Fred T. Goldstein*

FTG Software Associates, P.O. Box 579, Princeton, NJ USA 08542

ABSTRACT

Optical coatings are subject to random and systematic errors. Assuming unvarying dispersion, least-squares fitting of measured spectra provides means to solve for non-gross thickness errors. Unlike coating design, in which many acceptable and nearly equivalent solutions are possible, inverse-synthesis requires the unique and correct solution.

We introduce a 'Gedankenspektrum' (thought spectrum) method for determining the range and types of spectra required for a correct solution. Starting with an ideal design, we simulate production errors and then calculate the spectrum. Returning to the original design, we solve for the layers corresponding to the modified spectrum. Finally, if each layer is close to its known value, inverse-synthesis is successful; otherwise it fails. The process is repeated until the statistics become clear. Reliability depends on the type of design, number of layers, and measurement specifics. Most importantly, reliability increases markedly when measurements at non-normal incidence are included. This indicates the insufficiency in the (usual?) practice of measuring optical coatings solely according to pass/fail criteria.

A second 'Gedankenspektrum' method helps decide which spectral measurements and film thicknesses are required for determining n&k in single films, particularly metals. Starting with given dispersion values, random noise is added to calculated spectra, thereby simulating measurement conditions. We then solve for n&k and compare to given values.

1. INTRODUCTION

Consider two different thin film designs. Since the resultant spectra will not be perfectly identical, there is the possibility of uniquely deducing layer construction by inverse-synthesis. In practice this does not work because we are always limited in the accuracy and range of measurements. An extreme example is a normal incidence spectrum at a single wavelength; while that value might be suitable for pass/fail quality assurance purposes, we can deduce nothing about correcting the deposition process should the coating not meet requirements.

Coating errors can be gross, random, or systematic. Gross errors, such as a failure to deposit all layers or substituting half waves for quarter waves, are often discoverable by visually comparing spectra. Random and systematic errors can be analyzed by inverse-synthesis using least-squares fitting. Hopefully we can reduce random errors by better process control and can compensate for systematic errors by further analysis.

2. RELIABILITY OF INVERSE-SYNTHESIS

Inverse-synthesis is quite similar to coating design, except that measured results are the optimization targets. Starting with our initial design, our optimization targets are measured spectra. Unlike coating design where several thin film designs can meet specifications (some better than others) , inverse-synthesis requires the correct and unique solution.

2.1 26 Layer Design Example

We illustrate the procedure with a 26-layer laser output coupler design (T = 2% from 450 to 650 nm): Substrate (1.52) 31.048H 58.773L 49.156H 82.213L 51.563H 80.259L 51.115H 82.1L 53.466H 86.389L 56.066H 90.019L 58.318H 94.767L 64.937H 119.445L 70.047H 100.034L 64.521H 122.432L 76.715H 105.328L 77.837H 136.433L 72.492H 75.137L Air (1.0) where L is 1.46 and H is 2.3. Thicknesses are in nanometers. There was no particular reason to choose this design except that it was handy and seemed to have neither too few layers nor too many. The spectrum is shown in Figure 1. While the coupler is only used from 450 to 650 nm, initial results indicated that expanding the wavelength range would be useful in inverse-synthesis.

*fredg@ftgsoftware.com; phone +1 609 924-6222; fax +1 609 482-8060; http://ftgsoftware.com
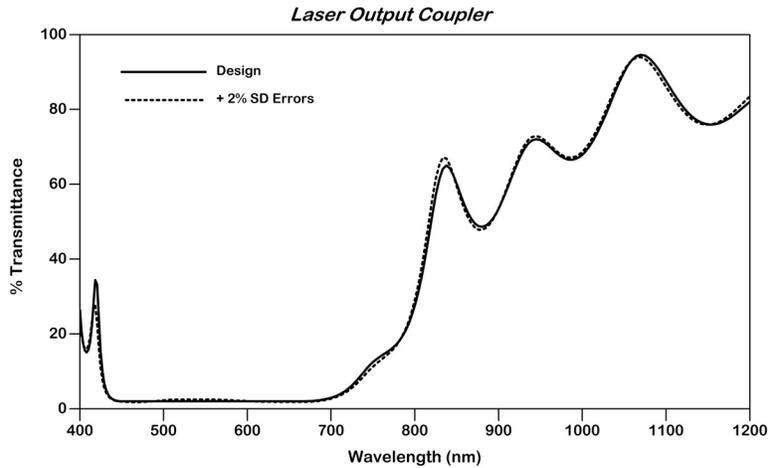
Fig. 1. Effect of random thickness errors in a 26-layer laser output coupler design.

The above figure might lead one to think that the design is quite resistant to thickness errors. Using our software's the zoom function reveals differently as can be seen in the next figure.
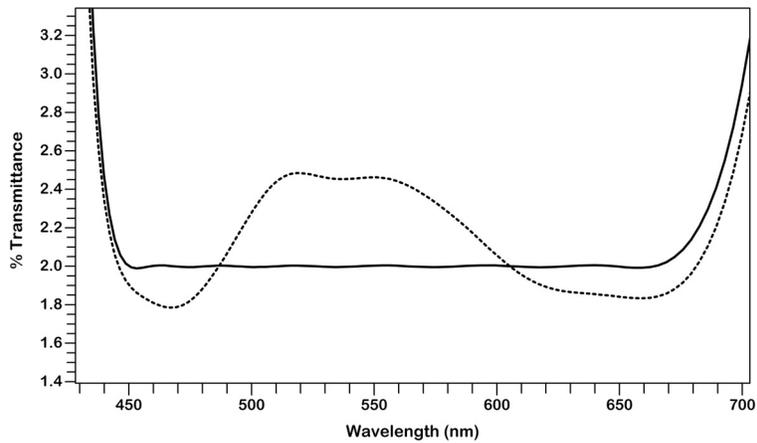

Fig. 2. Same graph as Figure 1 using zoom function.

2.2 Method

We calculate the reliability of inverse-synthesis by the following general method:

1. Starting with a given design, simulate production errors by generating a new design with random layer errors. We use percent errors herein, but absolute errors can also be utilized.

2. Calculate a spectrum (spectra) and convert to optimization targets.

3. Restore the original design and solve for the randomized design by DLS (damped least-squares) fitting.

4. If each layer is close to its known thickness (say within 0.5%), inverse-synthesis is considered successful, otherwise we have an invalid solution.

These procedures are implemented in our thin film design software through a built-in macro language compatible with *Microsoft* VBA (Visual Basic for Applications). As illustrated in the screenshot below, the core Basic language is supplemented by numerous host-specific functions, properties, and subroutines. While similar capability could easily be

built into the host design software, the macro language provides users with the ability to modify simulation procedures. For example, the pseudo-normal error distribution utilized here (CalcRand) might be replaced by a more sophisticated model. The code listed below works in *Microsoft* Excel when functions such as CalcRand are replaced with something like DesignObj.CalcRand where DesignObj is an external reference to the design software.

```
FilmStar BASIC - C:\Winfilm\Gedanken\Basic32\FilmSolve0 Code List.bas
File  Edit  View  Macro  Debug  Sheet  Help

Object: (General)                                Proc: Main

1   Option Explicit
    Option Base 1

    Sub Main
        Dim i%, k%, IterNG%, nLayers%, Design0$, qDesign!(), qDesc$(), qSolve!(), qType$()
        Const TestPC! = .5        ' verification value 0.5%
        Const Iter% = 10          ' iterations, change as required
        Design0 = Design          ' retain original design
        Angle = 0                 ' normal incidence
        For i = 1 To Iter         ' repeat Iter times
            Design = Design0       ' reassign original design
            CalcRand 0, 1          ' randomize layers, retaining randomized design
            GetLayers nLayers, qDesign(), qType$(), qDesc()
            SpecTargets  True, "T", 1, 0, "R"    ' convert spectrum to opti targets
            Design = Design0       ' reassign original design for optimizer
            Optimize               ' solve (DLS)
            GetLayers nLayers, qSolve(), qType$(), qDesc()
            For k = 1 To nLayers            ' compare layers to original
                If Abs(qSolve(k) - qDesign(k))/qDesign(k) > TestPC/100 Then
                    IterNG = IterNG + 1 ' fails
                    Exit For            ' exit the loop
                End If
            Next k
        Next i
        Design = Design0          ' restore original design for next iteration
        MsgBox "Confidence Level = " & CStr(100*(Iter - IterNG)/Iter) & "%", _
            vbInformation, "Inverse Synthesis 0°"
    End Sub
```

Fig. 3. Algorithm for computing the reliability of inverse-synthesis.

In practice, this code is supplemented by graphically displaying validity. The known spectrum is first plotted in blue. This is overlaid by the curve corresponding to the DLS solution. If that curve is green, the solution is valid (all layers within a given percent); if it is red, the solution is invalid. The exact spectrum and the solution spectrum are always (except for a pixel or two) exactly congruent. This is illustrated in the next graph which includes three overlapping plots. In our 26 layer example DLS calculations (subroutine Optimize) terminate when changes in the merit function (sum of [tDesign - tSolution]^2 at 221 wavelengths from 400-1200 nm) are 0.0001 or less.
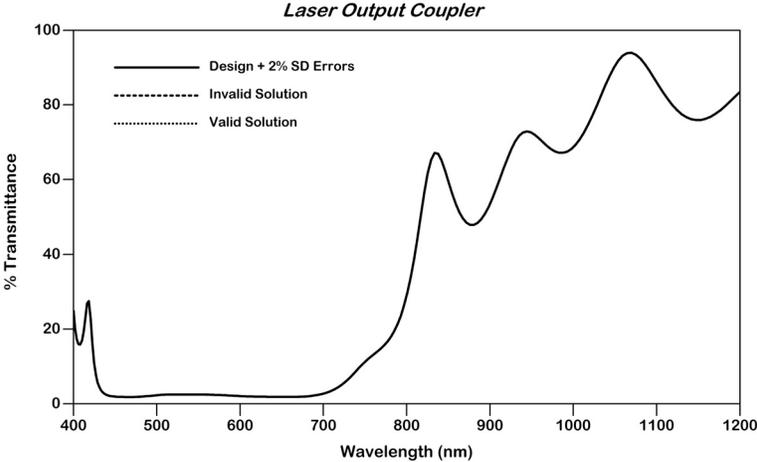

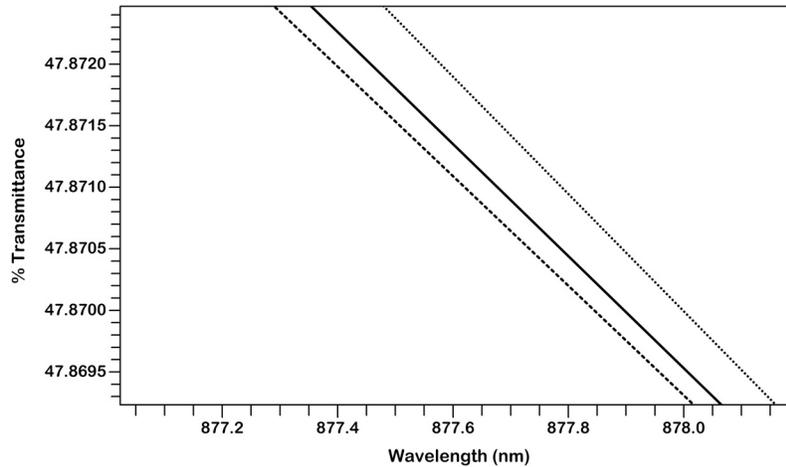Fig. 4. Overlapping spectra indicate that valid and invalid solutions cannot be distinguished.

Fig. 5. Same graph as Figure 4 with a zoomed region displayed.

As seen in Figure 5, differences between solutions are meaningless in relation to spectroscopic accuracy.

2.3 Results

Using the range 400-1200 nm and an accuracy criterion of 0.5% we determined that reliability is essentially zero. *Adding spectra at 45° increases reliability to ~100%.* Using the actual performance range 450-650 nm, reliability at either 0° or 0-45° is zero. The dramatic improvement from adding 45° values was surprising.

Reliability depends on the type of design, number of layers, magnitude of errors, measurement range, angle, and accuracy criterion. Repeating the analysis for a four layer 450-750 nm AR coating with layer StdDev = 5% gave 100% reliability (0.5% layer test) for calculations over the range 450-750 (0°). When StdDev = 20%, reliability becomes 56% (0°); expanding the range to 400-1200 nm gives 76% (0°) and 92% (0-45°).

3. N&K DETERMINATION

Our second Gedankenspektrum method relates to the problem of determining n&k from measured spectra. The literature contains a plethora of papers on this subject. How does one select a suitable method and verify its applicability and accuracy? Our proposal is to generate spectra with similar materials of known dispersion and see whether the correct solution (known n&k file) is deduced. We want to answer questions such as

- How thick a TiO2 film is required for confidence in the envelope method? How accurate are the k values computed by this method?

- Do we need reflection and transmission spectra, or is reflectance sufficient for Tauc-Lorentz analysis?

- Can we get better solutions for metals if we include measurements at non-normal incidence?

3.1 Method

Given a dispersive file, we create a Gedankenspektrum and solve for n&k. (It might be interesting to ask a colleague to determine the solution.) We then compare the solution with known n&k values. In our experience, the task is not complete because the precision of calculated spectra will be higher than that measured in practice. While the computer might happily distinguish n&k for 0.001% and 0.002% transmittance, the measurements may have RMS noise of 0.01%.

It is therefore important that we repeat our n&k calculations with computed spectra containing simulated noise. As a first approximation, we will assume that the noise is independent of wavelength. Here we assume that we have normally-distributed random values. This is easily accomplished in our BASIC macro language. As shown below, Excel provides an easy way to add random noise using an algorithm that we originally found in an IBM Fortran manual. RAND() is a built-in Excel function that returns uniformly distributed numbers in the range 0 to 1.

Fig. 6. Excel workbook illustrating function for adding noise to calculated spectra

The effect of 0.2% SD noise is shown in the following dispersion plots. The original Sopra file cannot be distinguished from our least-squares solution. While k values are hardly affected, n values show significant scatter (solid triangles in Figure 7.). Our Gedankenspektrum simulation (30 nm Ag film on BK7) included normal incident reflectance and transmittance spectra plus the same at 45° P and S polarization. Would normal incidence be sufficient? (In this case the inclusion of 45° spectra reduces n variations.) Will the same method work with thicker or thinner films? These are questions that must be answered before analyzing actual measurements.
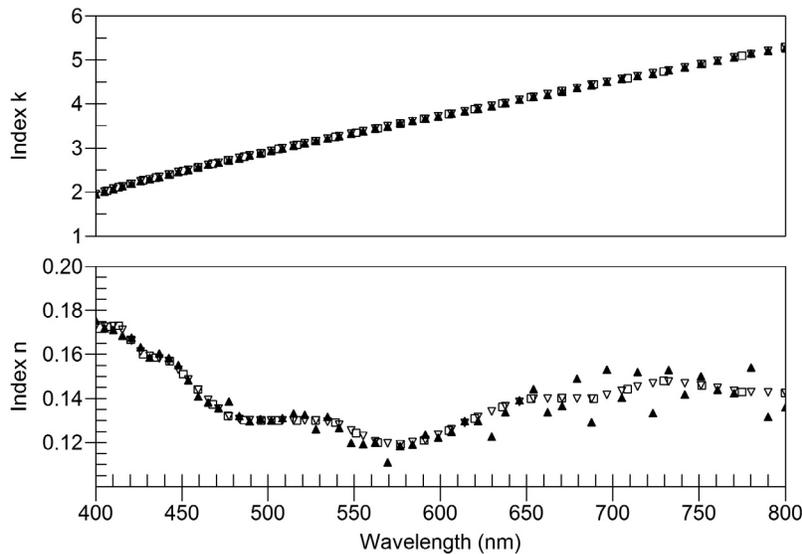

Fig. 7. Effect of 0.2% SD noise added to 30 nm Ag spectra. Open symbols are the original Sopra values (square) and DLS Gedankenspektrum solution (triangle). Solid triangles correspond to spectra with S.D. = 0.2%.

We do not wish to imply that high measurement accuracy is required in all cases. In Figure 7 (above) we solved for Ag n&k by least squares fitting spectra at each wavelength, using the last solution as starting point for the next wavelength. Here each n,k value depends on the accuracy of its corresponding R,T data.

When using a parametric fit[1] useful n,k values are possible with noisy data. This is illustrated below in Figure 8 with actual measured data. If one mentally averages the spectrum, the data look promising. (With so much noise, averaging the spectrum by a boxcar or Savitzky-Golay method is not advised.) Here we used a Lorentzian fit with 4 coefficients.
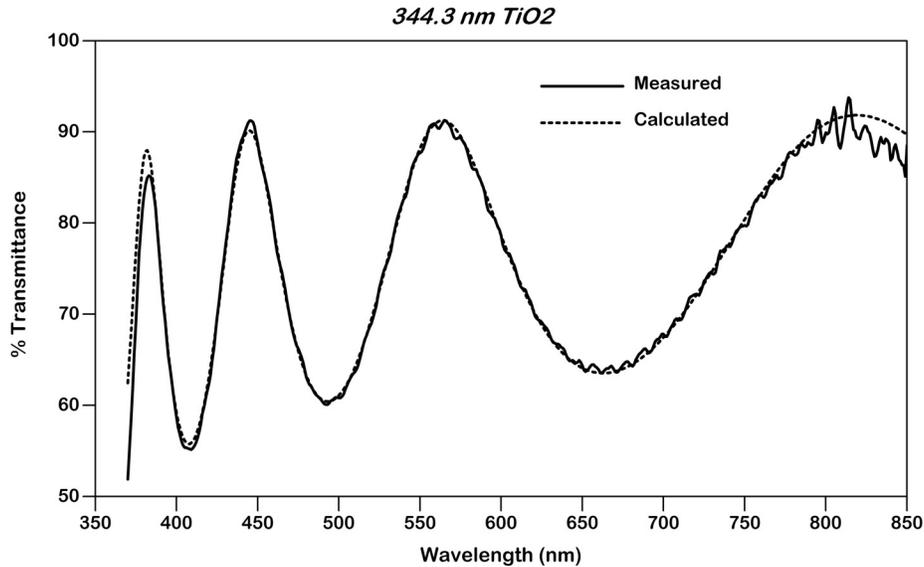
5

Fig. 8. Lorentzian fit to extremely noisy measured data from a defective spectrophotometer.

4. DISCUSSION

The work described in this paper is not intended to offer conclusions about particular designs or film materials. Rather, we have offered general ideas which need to be applied in particular cases.

4.1 Inverse-synthesis

We have described a method for estimating the reliability of inverse-synthesis; the method can be applied to all types of coatings. It seems clear that coating facilities can benefit greatly from upgrading measurement technology well beyond the minimum required for pass/fail analysis.

It is important to understand the characteristics of one's measurement apparatus. A nagging issue is whether commercial spectrophotometers are capable of sufficiently accurate non-normal incidence measurements. As inverse-synthesis is essentially a parametric fit, we assume that random measurement errors (e.g. noise) are not as important as systematic errors (e.g. drift in single-beam spectrometers). A suggestion for future work is to add wavelength-dependent measurement errors (systematic and random) for scanning, diode-array, and FTIR spectrometers.

While 100% theoretical reliability does not guarantee 100% reliability in practice, we believe that failure of the theoretical simulation guarantees failure with measured data.

4.2 n&k determination

Here we have more questions than conclusions.

Are both reflection and transmission measurements required? What is the optimum film thickness for n&k analysis in metals? in dielectrics? Which materials are amenable to automatic analysis with an off-the-shelf reflective n&k analyzer based on a single dispersive model? In which cases are diode-array spectrophotometers suitable for n&k analysis? In which cases are ellipsometric methods superior?

These are all questions that benefit from Gedankenspektrum methods.

---

[1] Dobrowolski, J. A., Ho, F. C. and Waldorf, A., "Determination of optical constants of thin film coating materials based on inverse synthesis", Applied Optics 22, 3191-3200 (1983).