Constrained optimization of band edge filter matching layers

Ronald R. Willey

Consultant, 6 Hop Brook Road
Brookfield, CT 06804, USA

ABSTRACT

A constrained optimization design procedure is described which gives good control of the spectral position of a filter edge and simultaneously optimizes pass band transmittance. The underlying principle of our previous study was to use constant level monitoring (CLM) and position that constant layer termination photometric level for the least sensitivity to photometric and other layer termination errors. Additional layers are needed between the substrate and the periodic stack to bring the layer termination to the ideal level and also provide the antireflection coating for the pass band of interest. The requirement can be stated as: the preliminary layers must move the reflectance phase at the monitoring wavelength from that of the substrate to that of the start of the periodic stack needed for CLM. The constraints are that the magnitude and phase values at the end of the deposition of the preliminary layers satisfy these specific requirements. The constrained optimization can vary both the pre- and post-periodic matching layers (without varying the periodic stack itself) while attempting to meet the transmittance targets and simultaneously satisfy the constraints. When this is done, the resulting design has optimized transmittance and satisfies the required constant level optical monitoring conditions for the most reproducible results in production.

Key Words: constrained optimization, constant level optical monitoring, optical monitoring errors, antireflection, matching layers, design of experiments

1. INTRODUCTION

Edge filters generally have a blocked band and pass band of interest. The transition between these bands is the edge. High transmittance in the pass band is usually desired. We have previously[1] described how to obtain the most stable results near the spectral edge of the filter. This paper addresses a design procedure to give optimal control of the edge position and simultaneously optimize the pass band transmittance by the constrained optimization of the matching or antireflection (AR) layers on both sides of the periodic stack which creates the edge filter.

The underlying principle of the previous study was to use CLM as described by Macleod and Pelletier [2] and position that constant layer termination level for the least sensitivity to photometric and other layer termination errors. It was shown[1] that the optimum layer termination levels were generally slightly above 50% reflectance. Such levels are not generally a natural consequence of an edge filter design which is intended to use CLM. A set of layers between the substrate and the periodic stack is needed which brings the cut level up to this >50% point and also provides the AR coating or matching layers needed for the pass band of interest. The preliminary layers must move the reflectance phase at the monitor wavelength from that of the substrate to the specific reflectance of the start of the periodic stack needed for CLM. The required phase at the end of the preliminary layers is usually either zero or pi. The constraints are that the magnitude and phase satisfy these specific values at the end of the deposition of the preliminary layers. Matching layers after the periodic stack also provide the interface to the final medium (usually air) in such a way as to minimize the reflection effects of that interface in the pass band. These post-stack layers can often be designed before the constrained pre-stack layers by unconstrained optimization over the band of interest. If a small number of post-stack layers are used which give a residual reflection that is significant with respect to the pre-stack layers, it may be beneficial to optimize the post-stack layers simultaneously with the pre-stack layers and constraints for the best results. On the other hand, if a large number (>4) of post-stack layers are used, that set of layers can be designed only once for a small reflectance value over the band and kept constant while the pre-stack layers are designed.

Goldstein[3] described the use of constrained optimization in optical coating design. The constrained optimization can vary both the pre- and post-periodic sets of matching layers (without varying the periodic stack itself) while attempting to meet the reflectance and/or transmittance targets and simultaneously satisfy the constraints.

Part of the EUROPTO Conference on Advances in Optical Interference Coatings
Berlin, Germany • May 1999
SPIE Vol. 3738 • 0277-786X/99/$10.00

We have recently reported[4] on a study which determined the minimum average percent reflection (Rave) that can be expected in a passband as a function of the bandwidth and the total number of matching layers. This work was without the above constraints applied, and as one might expect, that Rave will generally be greater when additional constraints are included.

2. GENERAL DESIGN PROCEDURE

Figure 1 illustrates a long wavelength pass (LWP) filter with a blocking edge at 8568 cm^{-1} and a pass band from 4200 to 8200 cm^{-1}. This design is a periodic stack of (.5H 1L .5H)6 at 10000 cm^{-1} plus six (6) pre-stack and ten (10) post-stack matching layers, where the indices are L = 1.46, H = 2.2, and the substrate is 1.52. CLM is illustrated in Fig. 2 with the layer termination level of layers 9 through 20 slightly above 50% reflectance. Two negligibly thick layers (7 and 8) of high and low index have been inserted in the design to show the break point from the pre-stack layers to the periodic stack.

The first part of the requirement for a preliminary set of layers is illustrated in the reflectance circle diagram of Fig. 3. It can be stated as: the locus of the reflectance phase versus deposition thickness of the preliminary layers must move from the reflectance of the substrate to the specific reflectance of the start of the periodic stack needed for CLM at the monitoring wavelength. The monitoring frequency (cm^{-1}) and effective index of refraction at the start of the periodic stack have been determined by the techniques described previously[1] to be 8607 cm^{-1} and 0.42, respectively.

In this case with a substrate of index 1.52, the reflectance would start at $r = -.20635 + i0$ (R = 4.258%) and move clockwise with the deposition of successive matching layers to the point $r = .4084 + i0$ (R = 16.68%) which has an effective index of refraction of $.42 + i0$. The required phase at the end of the preliminary layers is usually either zero (as in Fig. 3) or pi. The reflectance magnitude and phase therefore must be constrained in the optimization to conform to these specific values at the end of the deposition of the preliminary layers. This makes it possible to have the constant layer termination level for the periodic layers 9 through 20 illustrated in Fig. 2. The periodic section, where CLM is used, might have many more layers than the 13 illustrated here (for simplicity), and the pre-stack layers might be more than six.

3. SPECIFIC DESIGN PROCEDURE

An optical thin film optimization tool is needed which has the ability to impose constraints while optimizing. In the work reported here, we have used FilmStar[5] and the details reported refer to nomenclature used by that tool.

One of the goals is to design matching layers before and after the periodic stack which minimize the reflection in the pass band. This is an ordinary thin film design task which can be handled via: a starting design, performance targets, optimization variables, and an optimization routine. The extraordinary task is to also constrain the reflectance amplitude and phase to specific values at the end of the first set of matching layers. The constrained optimization does not vary layers 7 through 21. The free variables are layers 1-6 and 22-31. The targets were set to minimize the reflection from 4200 to 8200 cm^{-1}. We chose as a starting design: (.5H 1L .5H)15, where L = 1.46 and H = 2.2. After this "group design" was expanded to a "layers design," it was optimized (using the constraints) by varying the first 6 and last 10 layers.

It is necessary to use the Workbook spreadsheet capability of FilmStar to implement the necessary constraints. When optimizing from the Workbook, five named cells or ranges are key to the computational procedure which is executed. These are: **Design, Macro, Objective, Constraint, and DataMarker**. **Design** indicates the section of the worksheet where the current design is copied. **Macro** defines a sequence of operations which occur during each iteration of optimization. **Objective** (merit function) is the number to be minimized by the optimization. This is ordinarily the weighted average of reflectance or transmittance over some spectral band (range of worksheet cells). **Constraint** defines multiple conditions which will be forced to satisfaction as the optimization progresses. **DataMarker** defines the upper left of the spectral data array which is updated during each iteration.

The Macro in this case was as follows:

```
AxesOpen CNSTR1;LayersCopy;Calculate;Basrun C:\winfilm\basic\DESPLITU.bas;DesignPaste;Calculate;Basrun
C:\winfilm\basic\DESCOPYU.bas;DesignPaste;
```

This performs the sequence described next. **AxesOpen** loads axis definition file, **CNSTR1**, which defines the spectral data to be calculated from the current design. This might be the axes defined in Fig. 1 where the reflectance is evaluated from 30 to 10000 cm^{-1} in some specified increment. In the particular case described here, we chose an increment which caused the monitoring frequency (8607 cm^{-1}) to be one of the sample points and therefore a cell in the Workbook that can be addressed for constraint calculations. In this case, we were particularly interested in the reflectance phase at 8607 cm^{-1}. The next macro operation is to execute a **LayersCopy** command to copy the design to the defined **Design** place on the worksheet. Then a **Calculate** command is executed to evaluate the design at the spectral points defined by the axis file. These are automatically copied to the worksheet area defined by the **DataMarker**.

A basic program with the name **C:\winfilm\basic\DESPLITU.bas** is then executed. This program is as follows:

```
Sub Main
    WbCopy "$K$12:$K$42"
    WbPaste "$L$12:$L$42"
    WbCopy "$L$12:$L$17"
    WbPaste "$M$12:$M$17"
End Sub
```

This copies the whole design to the clipboard and then pastes it to an adjacent column on the worksheet for future use. It then copies to the clipboard the layers (6, in the case of Figs. 1-3) up to the point where the constraint is imposed on the reflectance phase, and then pastes it to another adjacent area. The next Macro command, **DesignPaste**, pastes the abbreviated design which is still on the clipboard onto the design area of the worksheet. The **Calculate** command is executed which evaluates this abbreviated design with respect to the axes definition and stores the results on the worksheet to the right of the previous evaluation of the whole design.

The **Objective**, which in this case was the average of the reflectance from 4200 to 8200 cm^{-1}, is calculated by the worksheet as the average over those cells where these reflectance values lie. A spectral weighting can be applied by making another column elsewhere on the worksheet which is the product of the calculated values times the spectral weighting function. The sum or average of this new column would then be the definition in the **Objective** cell.

The **Constraints** or violations thereof can now be evaluated by the worksheet from two cells of the second **Calculation** results with the abbreviated design. The cell with the reflected phase at 8607 cm^{-1} is compared with the target value for its constraint, and the cell with the reflected amplitude is compared with its constraint.

Before going on to the next iteration, it is necessary to restore the whole design. This is done by the macro commands:

```
Basrun C:\winfilm\basic\DESCOPYU.bas;DesignPaste;
```

This basic program is simply:

```
Sub Main
    WbCopy "$L$12:$L$42"
End Sub
```

Here, the whole design which was saved is now copied to the clipboard. The **DesignPaste** command puts it back in the correct position on the worksheet.

This completes the iteration and the cycle is repeated until the optimization procedure terminates itself or is terminated by the designer.

4. RESULTS

The convergence of this design procedure has been generally satisfactory. However, it not as rapid as unconstrained optimization and appears to be more vulnerable to falling onto "local minima". We have found two potential pitfalls to avoid. One is that the number and indices of preliminary layers to be optimized must be sufficient to reach the reflectance and phase of the constraint point from the starting point. A single layer will almost never be enough and three may occasionally be sufficient. Six or more layers are more commonly successful and appropriate when attempting to minimize the reflectance over a broad pass band. Figure 4 shows the Rave results of a systematic set of optimizations of pre-stack layer designs with 4 to 11 layers and at bandwidths of 0.2, 0.4, and 0.8. The bandwidth is defined as the range of wavenumbers in the pass band divided by the range from zero to the center of the block band (in this case 10000 cm^1). The example in Figs. 1-3 has a bandwidth of 0.4. The AR behavior here has been found to be generally consistent with our earlier findings[4]. The second pitfall is the phase discontinuity found at the extremes of plus or minus pi when constraining the phase to pi. We overcame this by constraining the square of the phase to be equal to pi squared.

The resulting Rave's from the above optimizations as a function of the two variables (total number of pre- stack (AR) layers from 6 to 11 and bandwidth from 0.2 to 0.8) were treated as Historical Data using design of experiments (DOE) methodology as described by Schmidt and Launsby[6]. When this data is processed by standard DOE statistical software[7], the results can be readily illustrated in two and three dimensional graphic plots. The software also provides the coefficients for equations to calculate any point on these surfaces that have been statistically fit to the data to the third order including interactions of the variables. The resulting equation is:

$$\mathrm{Rave} = 7.6455 - 0.4641N - 16.423B - 2.127NB + 57.71B^2 - 35.2B^3 + 0.139N^2B. \qquad (1)$$

Here B is the bandwidth and N is the number of pre-stack layers. This equation was used to generate the dotted lines in Fig. 4 to compare with the "experimental" data of the solid lines. In our recent work[4] on unconstrained optimizations of similar long wave pass filters (LWP), we found the following equation to be a good fit to the optimizations of that work:

$$\mathrm{Rave\ (LWP)} = 2.1678 - .7247N + 5.0606B + .0441N^2 - .0007N^3. \qquad (2)$$

When these two equations are used to compare the number of extra layers required to satisfy the constraints and achieve similar Rave results, it is found that approximately 3 extra layers are required. If the bandwidth is greater than approximately 0.3, this number 3 varies by only a small fraction of a layer with bandwidth and number of layers. At bandwidths smaller than 0.3, six (6) layers may be needed for good constrained results; whereas only two might be adequate for an unconstrained AR.

5. CONCLUSIONS

We have previously[1] shown, graphically and with equations, how to find the proper monitoring wavelength and effective index needed to achieve stable control of edge filter deposition by constant termination level optical monitoring. We have shown here how to use that information to complete a design and monitoring scheme which is maximally robust and simultaneously controls a blocking edge position and pass band transmission. An additional three (3) layers is typically needed to satisfy the optimal monitoring constrained condition for CLM as compared to not using optimal CLM which might lead to far from optimal results.

6. REFERENCES

1. R. R. Willey and D. E. Machado, "The variation of band edge position with errors in monitoring layer termination level for long and short wave pass filters," presented at the Optical Interference Coatings Conference in Tucson, AR in June of 1998 and submitted to *Applied Optics*.
2. H. A. Macleod and E. Pelletier, "Error compensation mechanisms in some thin-film monitoring systems," *Opt. Acta* **24**, 907-930 (1977).
3. F. T. Goldstein, "Constrained optimization with user-specified functions," Paper WG1 at the Optical Interference Coatings Topical Meeting, June 7-12, 1998, Tucson, AR
4. R. R. Willey, "Estimating the Reflection Losses in the Passband of Edge Filters," *Soc. Vac. Coaters 42nd Tech. Con. Proc.*, Paper O-22 (1999).
5. FilmStar[TM], FTG Software Associates, P.O. Box 579, Princeton, NJ 08542
6. S. R. Schmidt and R. G. Launsby, Understanding Industrial Designed Experiments, Sec. 3.8, Air Academy Press, Colorado Springs, 1994.
7. DOE KISS[TM], Ver. 97 for Windows, Air Academy Associates (and Digital Computations, Inc.), Colorado Springs (1997).

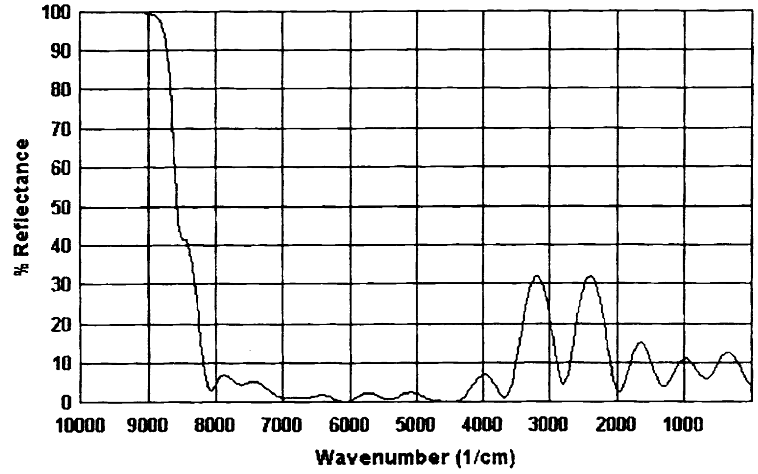

Fig. 1. LWP filter design with a periodic stack of (.5H 1L .5H)6 at 10000 cm^{-1} plus 6 pre-stack AR layers, where the indices are L = 1.46, H = 2.2, and the substrate is 1.52.

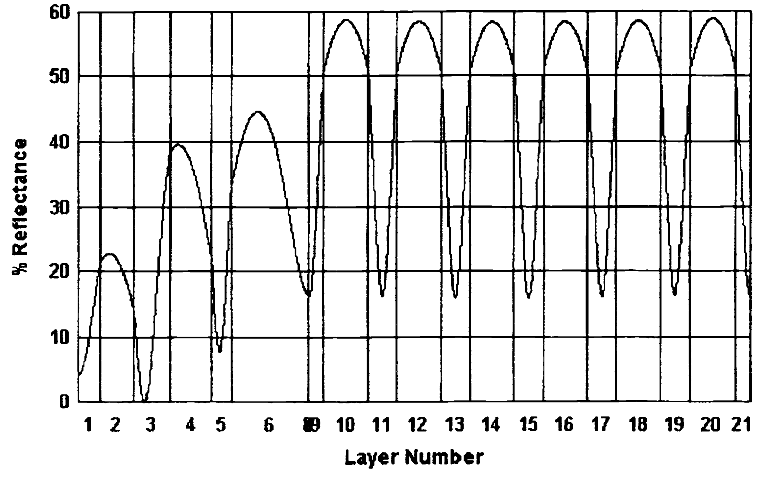

Fig. 2. Constant Level Monitoring at 8607 cm^{-1} at 8607 cm^{-1} of design illustrated in Fig. 1. Two very thin layers (7 and 8) of high and low index have been inserted to show the break point from the pre-stack layers to the periodic stack.

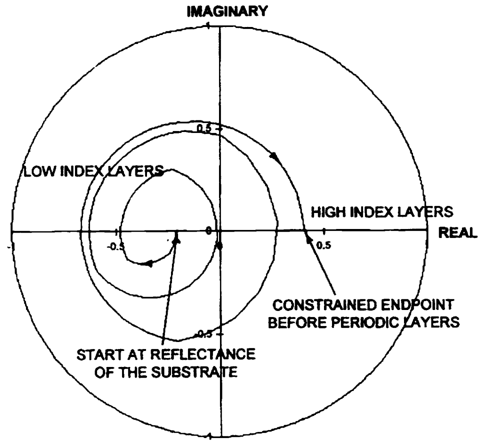

Fig. 3. Amplitude reflectance diagram of the first 6 layers of the design in Fig. 1 at 8607 cm^{-1}. The locus of the reflectance phase versus thickness of the pre-stack layers moves from the substrate to the start of the periodic stack for CLM.

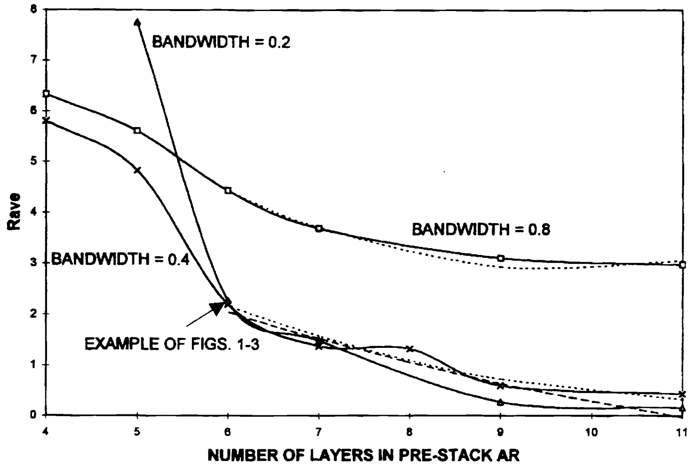

Fig. 4. The Rave results of a systematic set of pre-stack layer designs at bandwidths of 0.2, 0.4, and 0.8. Solid lines with symbols for specific designs. Dotted lines generated by equations from statistical fit to results from 6-11 layers.