Variation of band-edge position with errors in the monitoring of layer termination level for long- and short-wave pass filters

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Optical monitoring of periodic thin-film stacks by the termination of each layer at the same constant photometric level has certain advantages. One of these principal advantages is the error compensation effect in the vicinity of the monitoring wavelength. In this study, we examine, by simulation, the effect of an error in the knowledge of the absolute value of the photometric termination level on the probable stability in the manufacture of the edge position of a blocked band. The results include equations that allow the determination of the appropriate values of parameters associated with the optimum termination levels to minimize the effects of such errors. © 1999 Optical Society of America

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1. Introduction

The goal of the deposition of layers in a thin-film optical coating is to achieve an adequately reproducible result from each coating run. Optical monitoring of layer thickness is generally favored when it is optical performance that is the required result. Some designs such as narrow-bandpass filters, as shown by Thoeni,[1] are mostly dependent on the optical thickness, whereas others such as beam splitters are more dependent on the index of refraction of the layers. Thoeni showed that the edge of a long-wavelength pass (LWP) or short-wavelength pass (SWP) filter such as shown in Fig. 1 depends on both optical thickness and index. In this research we deal more specifically with the control of these LWP and SWP edge positions.

If the photometric level of transmittance and reflectance from the optical monitor of the part being coated is accurately known during the deposition of a periodic stack, then both the optical thickness and the index of refraction (and thereby the physical thickness) can be calculated. Because the photometric level is not usually known as accurately as might be desired, it is beneficial to attempt to minimize the effects of errors in the absolute photometric level by the choice of the details of the monitoring strategy.

Macleod and Pelletier[2] showed the benefits of constant level monitoring for periodic layer structures; Zhao[3] expanded on the technique; and Willey[4] summarized and applied the methodology. Figure 2 shows such a monitoring strategy in which each of the periodic layers are terminated when the photometric level reaches 53%. The term level monitoring has come to be used more generally to mean terminating layers at some photometric level other than the inflection or turning points of the monitor signal. Here we are discussing the more specific constant level termination point monitoring as illustrated in Fig. 2.

We previously[5] pointed out that the greatest sensitivity of change in reflectance or transmittance of the monitor signal with change in coating thickness occurs when the reflected intensity R equals 36%. Macleod and Pelletier[2] showed how the position of the monitoring wavelength with respect to the band edge changed this sensitivity. Zhao[3] showed how the error compensation effects are most beneficial near the monitoring wavelength as in the classical case of monitoring a narrow-bandpass filter at its center wavelength. We encountered disappointing results using this strategy to monitor an edge filter at a wavelength somewhat removed from the edge. The study reported here makes apparent the major cause

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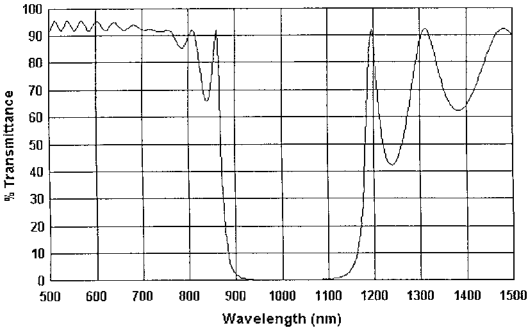

Fig. 1. Spectral transmittance of a SWP filter (0.5*L* 1*H* 0.5*L*)10 quarter-wave optical thicknesses at 1000 nm used for simulations of this research. *H* is index 2.2 and *L* is index 1.46.

of the problem. That is, the error in the knowledge of the absolute photometric level of the monitor signal has an increasingly more harmful effect as the monitor wavelength is farther from the band edge. As a consequence of this observation, we now choose to monitor as close to the edge as practical, and this implies layer termination levels slightly above 50% *R* as opposed to the 36% result of earlier studies. We used simulation techniques, as described below, to reach these conclusions, and we developed equations to aid the design engineer in setting up such monitoring conditions.

2. Preparations for Constant Level Monitoring

The task of preparing for constant level monitoring is to find the effective index underlying the periodic layers that will yield the constant photometric level desired for layer termination and the monitor wavelength that is required. Alternately, the task of preparing for constant level monitoring at a specific monitor wavelength is to find the effective index and layer termination level that will give constant level monitoring at the wavelength required. Equations to aid in finding these values are given below.

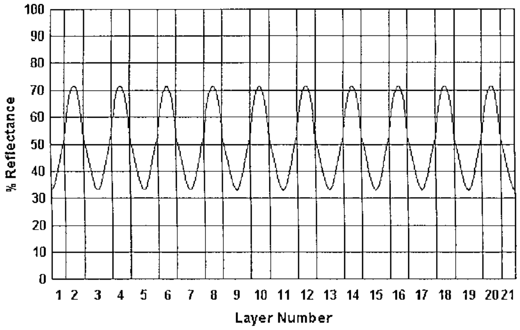

Fig. 2. Simulated monitoring trace in which each of the periodic layers are terminated when the photometric level reaches 53%. This is monitored at 878.6 nm on an effective index of 0.2593.

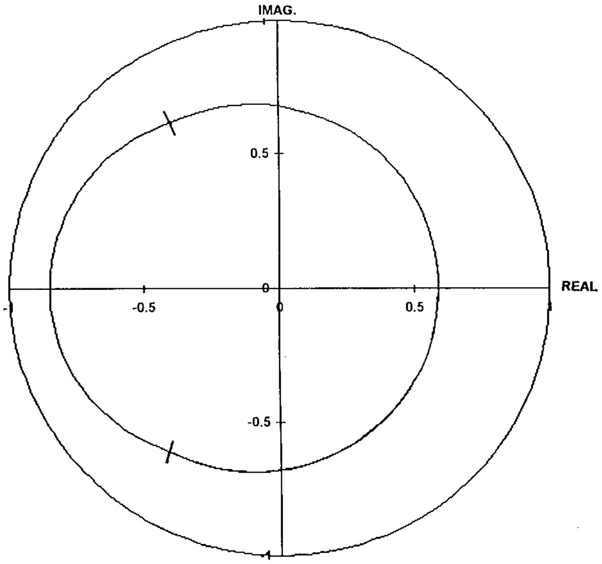

Fig. 3. Locus on a reflectance amplitude versus reflectance phase or circle diagram of the monitoring trace represented in Fig. 2 to achieve the desired result of Fig. 1.

The monitoring curve represented in Fig. 2, which is used to achieve the result desired in Fig. 1, can be seen in the circle diagram Fig. 3. These diagrams, as described in detail by Apfel,[6] are the reflectance amplitude and phase versus thickness of the coating as it would be deposited from the start of each layer to its termination. If the design is of the form (0.5*L* 1*H* 0.5*L*)10 with the indices of *H* and *L* equal to 2.2 and 1.46, respectively, as in Fig. 1, the reflectance amplitude needs to start at the point to the right of the origin in Fig. 3 where the locus intersects the real axis. This is the point where the reflectance amplitude ρ is equal to $0.588 + i0$, implying a phase of zero. When starting from this point, the first eighth-wave layer of low index (at the wavelength of the center of the stop band, not the wavelength of the edge) terminates at the marked point in the lower left quadrant. The next quarter-wave of high index terminates at the point marked in the upper left quadrant. Most optical monitors measure reflected (or transmitted) intensity *R* (or *T*). It is necessary to discuss both reflectance amplitude ρ and reflected intensity $R = \rho\rho^*$ in this type of investigation. The termination points discussed above are where *R* is 53% (and ρ is 0.728). The circle diagram often can give more insight with respect to some of these processes.

If the design were (0.5*H* 1*L* 0.5*H*)10 for a LWP filter to be monitored near the edge between 1150 and 1200 nm, it would also be necessary to start where the locus crosses the real axis, but the effective index would be higher and the locus would begin with the high-index material. We confine our discussion here to the SWP filter cases, but the principles would be the same.

Because the substrate usually does not have an index equal to the required effective index, a preliminary coating of one or more layers must bring the reflectance amplitude point from the substrate to the desired start of the periodic structure. In a future paper we plan to discuss a technique to design such a coating that simultaneously acts as an antireflection coating for a given spectral band. In the case of a substrate of index 1.5, the reflectance would start at $\rho = -0.2 + i0$ and move by successive layers to the point $\rho = 0.588 + i0$, which has an effective index of refraction of 0.2593.

3. Methodology for the Design of Experiments

The experiments used here are simulations derived by calculating the properties of the designs with respect to specific variations of parameters. The principal tools used to gain an understanding of the relationships and sensitivities in the research reported here were those of design of experiments (DOE) methodology as described by Schmidt and Launsby[7] and implemented in the software DOE KISS.[8] With these standard tools, we are able to empirically find the equations and graphics of the required working relationships to adequate approximations for the intended purpose without recourse to the laborious derivations of rigorous mathematics.

The Box–Behnken type of DOE for three variables was chosen which uses the factors of layer termination level, high index, and low index. The results or responses as a function of these variables that were examined include edge wavelength, monitoring wavelength, effective index, and the reflectance at maximum and minimum turning points. The ranges of the variables chosen to represent common ranges used for visible and near-infrared coatings were 16–56% for the layer termination level, 1.8–2.6 for the high index, and 1.36–1.56 for the low index. The Box–Behnken design for such a configuration gathers data at the centers of the 12 edges that define the three-dimensional cube of these limits plus the center of the cube. Statistically, this allows the estimation of all linear and quadratic effects and all two-way interactions. Our preliminary studies showed that higher-order effects were not of significance to our goals. The DOE methodology uses the ranges given to establish the values of the three variables at three levels for the 13 experiments. A Box–Wilson or central composite design might also have been used, but the Box–Behnken was chosen because it can model all the quadratic and linear interactions, and the extremes of the experiments bound the region of interest in a cube.

We carried out 13 simulations using thin-film design software[9] to empirically find the effective index and monitor wavelength that would give constant level monitoring at the specific values of 16, 36, and 56% for the index combinations in the ranges given above. This also gave the maximum and minimum inflection or turning point reflected intensity levels as a result. The edge wavelengths were calculated directly from the design for the indices given. The DOE software was then used to perform a regression analysis to find the best fit of the data to the range of surfaces that can be modeled by the Box–Behnken design. Where coefficients were found to be statistically insignificant, they were dropped, and the analysis was rerun with the reduced configuration. The resulting coefficients were then used to generate surface plots of the results as a function of the variables, and equations were generated for the calculation of any point on the surfaces.

4. Results

As shown below, the most stable monitoring results are predicted to be with a layer termination level in the region of 53% reflectance when the materials are of index 1.46 and 2.3 (such as might be the case with SiO_2 and TiO_2). Equation (1) shows the variation of the necessary effective index with the high and low indices when the termination level is at 53%:

$$N_F = -0.07882 + 0.01522H + 0.2088L. \tag{1}$$

Here L and H represent the low and high indices of refraction, and K is the termination level in percent reflected intensity (%R). Equation (2) is for the general case at any termination level in the ranges used:

$$N_F = -0.624 - 0.00086K + 0.113H + 1.07L - 0.00184KH - 0.01625KL - 0.00021K^2. \tag{2}$$

Similarly, Eq. (3) shows how the monitor wavelength in nanometers varies at a 53% termination level with low and high index:

$$\lambda_{\mathrm{mon}} = 1112.4 - 337.9H + 180L + 51.202H^2. \tag{3}$$

Equation (4) is for the general case at any termination level:

$$\lambda_{\mathrm{mon}} = 1207.8 + 1.189K - 449.7H + 180L + 2.109KH - 0.0564K^2 + 51.202H^2. \tag{4}$$

The principal concern of this research is to have stable results from coating runs wherein the filter edge of interest has a reproducible offset from the monitor wavelength in the presence of possible errors in the absolute photometric level of the layer termination. We therefore focused on the change in the difference between the monitor and the edge wavelengths ($\Delta\lambda$) with the photometric termination level. It was somewhat surprising to find that the $\Delta\lambda$ is not a function of the low index of refraction, but only the termination level and the high index. In Figs. 4–9, L is set to 1.46.

Figure 4 shows a view of $\Delta\lambda$ as a function of termination level and high index. It is apparent that there is a valley or trough where the change in $\Delta\lambda$ with the termination level is zero. Figure 5 is an overhead or contour view with a line drawn approximately along the bottom of this trough. At such points, the effect of an error in the absolute photometric level of a constant level monitoring termination should have a minimal effect. That is the goal of this research.

Equation (5) represents $\Delta\lambda$ as a function of K and H because L was found not to be a factor:

$$\Delta\lambda = -109.03 - 1.00065K + 112.5H - 2.11KH + 0.0538K^2. \tag{5}$$

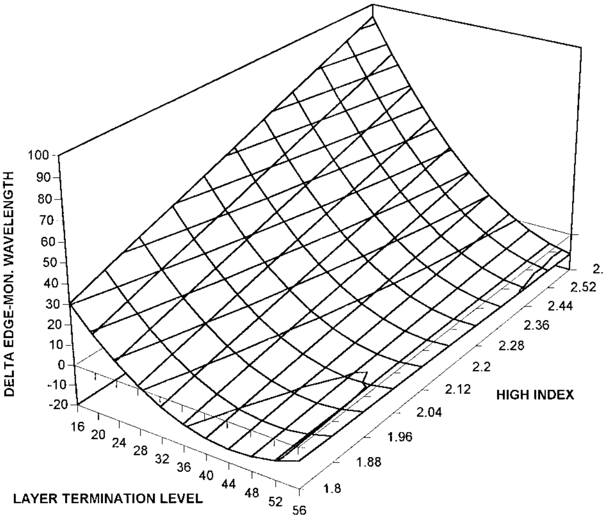

Fig. 4. View of Δλ, the difference between edge and monitoring wavelength, as a function of termination level *K* and high index *H*. Note the preferred area in the lower right where the rate of change with both *K* and *H* approach zero.

The derivative of this with respect to *K* is

$$\Delta\lambda/\Delta K = -1.00065 - 2.11H + 0.1076K. \quad (6)$$

When this $\Delta\lambda/\Delta K$ is set to zero, as in Eq. (7), the minimum sensitivity to photometric error would occur.

$$K = 9.294 + 19.61H. \quad (7)$$

This can be seen to be a linear function of *H* which would be 53% when $H = 2.229$. For the LWP case, the results are similar to everything discussed above and are given in Eq. (8):

$$K = -14.818 + 29.62H. \quad (8)$$

It can be found from Eqs. (7) and (8) that the optimum termination point is the same (56.5%) for both the SWP and the LWP filter when the high index is 2.4088.

Figures 6 and 7 illustrate the effects on the edge position of a 1% photometric calibration error at a layer termination level of 16 (and 15) and 53% (and 52), respectively. These effects were generated em-

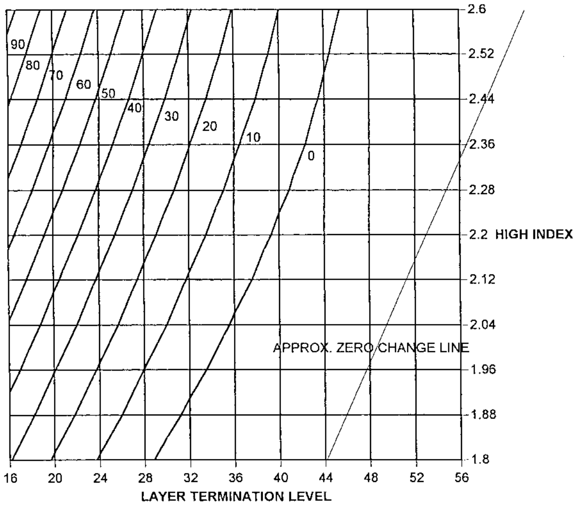

Fig. 5. Overhead or contour view of Δλ as in Fig. 4 with a line drawn along the region of zero change of Δλ with termination level.

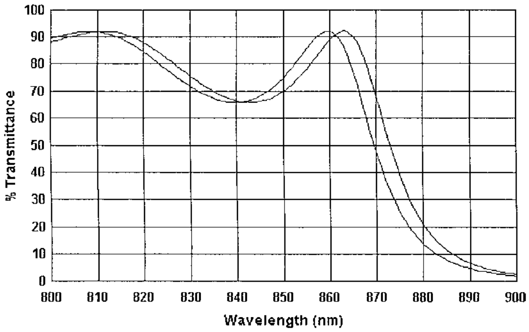

Fig. 6. Comparison of the edge position of the termination of each layer at 16% *R* with terminations having a photometric calibration error of 1% and thereby a termination level of 15%. This is an amplified view of the same coating as in Fig. 1 and was monitored at 808 nm.

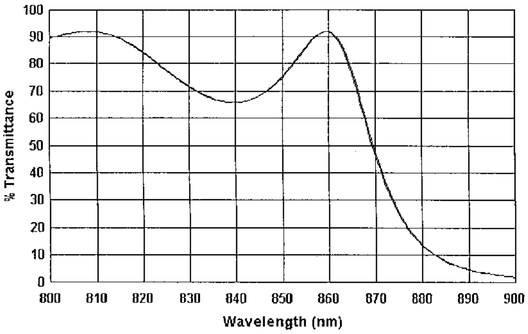

Fig. 7. Comparison of the edge position of the termination of each layer from the design of Fig. 1 at 53% *R* with terminations having a photometric calibration error of 1% and thereby a termination level of 52%. The monitoring wavelength is 878 nm.

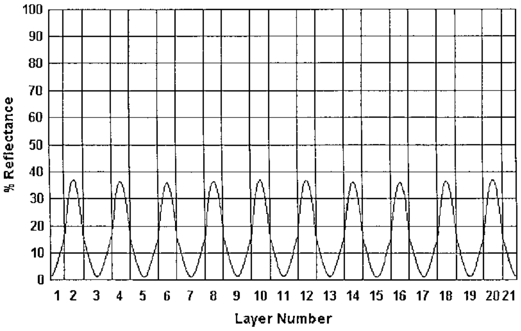

Fig. 8. Simulated monitoring trace (for comparison with Fig. 2) where each of the periodic layers are terminated when the photometric level reaches 16%. This is monitored at 808 nm on an effective index of 0.7826.

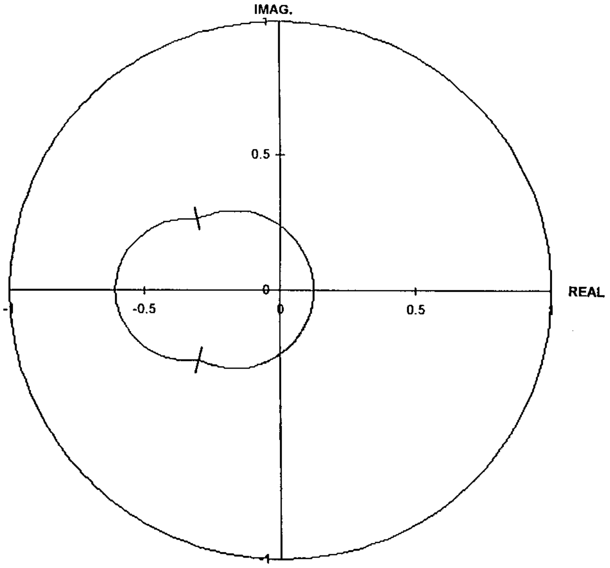

Fig. 9. Locus on a circle diagram of the monitoring trace represented in Fig. 8.

pirically by finding the film characteristics when the termination was 1% different from that intended. When the variables of $H = 2.2$, $L = 1.46$, and $K = 16$ and 53 are inserted into Eq. (6), we find that the errors predicted are 0.06 and 3.9 nm, respectively. This is in satisfactory agreement with Figs. 6 and 7.

Figures 8 and 9 show the predicted monitor trace and the reflectance circle diagrams for the 16% termination level case for comparison with those in Figs. 2 and 3 for the 53% case.

Auxiliary results are shown in Eqs. (9) and (10) where the $\%R$ of the maxima ($\%R_T$) and minima turning points ($\%R_B$) in constant level monitoring is a function of termination level, high index, and low index.

$$\begin{aligned}\%R_T = {} & -0.575 + 1.288K + 26.43H - 20.48L \\ & - 0.111KH + 0.283KL - 0.0074K^2 \\ & - 2.505H^2, \qquad (9)\end{aligned}$$

$$\begin{aligned}\%R_B = {} & 12.64 + 1.122K - 2.603H - 8.25L \\ & - 0.565KL - 0.00822K^2. \qquad (10)\end{aligned}$$

If the monitoring is to be near the other edge of the block band for a LWP, Eqs. (11)–(19) are applicable as Eqs. (1) and (10) are for the SWP.

$$\begin{aligned}N_F = {} & -2.175 + 0.1789H + 0.241L, \\ & \text{(at 53\% termination level)}, \qquad (11)\end{aligned}$$

$$\begin{aligned}N_F = {} & -0.425 - 0.0159K + 0.852H \\ & + 0.241L \\ & - 0.0127KH - 0.000343K^2, \qquad (12)\end{aligned}$$

$$\begin{aligned}\lambda_{\text{mon}} = {} & 1327.03 + 161.43H + 361.8L \\ & \text{(at 53\% termination level)}, \qquad (13)\end{aligned}$$

$$\begin{aligned}\lambda_{\text{mon}} = {} & 669 + 4.137K + 637.1H - 361.8L \\ & - 8.975KH + 0.1562K^2, \qquad (14)\end{aligned}$$

$$\begin{aligned}\Delta\lambda = {} & -597.37 + 4.49K + 441.1H \\ & - 8.975KH \\ & + 0.1513K^2, \qquad (15)\end{aligned}$$

$$\Delta\lambda/\Delta K = +4.49 - 8.975H + 0.3026K, \qquad (16)$$

$$K = -14.818 + 29.62H \qquad (17)$$

$$\begin{aligned}\%R_T = {} & -5.34 + 1.233K - 6.044H + 13L \\ & + 0.075KH - 0.00491K^2, \qquad (18)\end{aligned}$$

$$\begin{aligned}\%R_B = {} & 19.61 + 0.679K - 23.57H - 0.592KH \\ & + 0.0158K^2 + 8.026H^2. \qquad (19)\end{aligned}$$

We remind the reader that these studies were based on periodic stacks of equal quarter-waves at 1000 nm. The wavelengths would need to be scaled for particular cases other than 1000 nm, but otherwise the results would be the same.

5. Conclusions

The root cause of some of our earlier disappointments using constant level monitoring have been shown. It now appears that the best practice in monitoring edge filters composed of periodic structures is to monitor at a wavelength near the edge of interest which yields a reflected intensity layer termination level of 50–55% (or 45–50% if monitored in transmittance). We developed equations to select the most stable termination level [Eqs. (7) and (8)] and to find the proper monitoring wavelength and effective index [Eqs. (1)–(4) and (11)–(14)] needed to achieve such monitoring.

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