Simulation comparisons of monitoring strategies in narrow bandpass filters and antireflection coatings

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This study compares and quantifies the simulated effects of noise, index errors, and photometric level errors on different optical monitoring layer termination strategies. A computer program to simulate optical thin film monitoring has been written for this work. The study looked at these termination methods: quartz crystal monitoring, photometric level cut, two types of turning point termination, and percent of optical extrema monitoring. A narrow bandpass filter and a four-layer antireflection coating design were simulated as examples. © 2013 Optical Society of America

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1. Introduction

This work offers an alternative to previously reported simulators [1,2] for optical thin film monitoring. An optical thin film monitoring computer program in FilmStar Basic [3] was written to use in conjunction with the FilmStar Design [3] optical thin film software to simulate the effects of noise in the optical monitor signal, index errors, and photometric level errors on monitoring layer termination strategies.

Previous monitoring was done at a single wavelength (not broadband). The new software was written to allow testing of the percent of optical extrema monitoring (POEM) and a different turning point (TP) detection algorithm that has been inaccessible in the previous simulation programs.

The behavior of five different types/strategies of layer termination have been simulated and studied: quartz crystal monitoring (QCM), level cuts (LC), two TP determinations by change of slope (5 points) and parabola fit (P-Fit), and POEM. The TP termination algorithms described also include the ability to terminate at a specified physical thickness (PT) after the TP has been found (TP + PT) by either the 5-point or P-Fit method. The TP and TP + PT strategies depend upon finding the physical thickness at the TP by its “shape” (i.e., detecting the maximum or minimum (TP) of the near-sinusoidal monitoring curve by some curve-fitting algorithm).

2. Quartz Crystal Monitoring

QCM is known to be precise but not accurate, until it has been calibrated against a known optical thickness. QCM experts say that such a system can be reproduced to within 1% of its reading because of noise and other sources, such as calibration error or thermal effects. Issues such as plume variation can be improved by the use of multiple crystals around the parts being coated, and this further allows averaging and other error reduction techniques. When factors, such as crystal cooling water, radiation on the crystal, chamber wall deposits, chamber temperature and pressure, deposition rate variations, and adhesion to the crystal are considered, it is possible to reproduce 3%–5% of layer thickness. Such monitoring is common in the ophthalmic industry where the ability to reproduce may be somewhat better, and they generally achieve good results on four- to six-layer coatings. QCM can be useful in many applications, but there is no opportunity for it to compensate
for errors in previous layers. Therefore, the use of QCM alone is not likely to be satisfactory for demanding specifications with many layers, such as narrow bandpass filters (NBP). New software was written to accommodate random errors in QCM percent of thickness and also random absolute errors in thickness.

The simulations performed in this study assume that the technique of Schroedter [4] has been implemented in the monitoring system. Schroedter recorded the optical monitoring signal levels (Y values) at equal physical thickness intervals indicated by the QCM (X values) and calculated the predicted TP via a fitting algorithm. Historically, the monitor signal has been recorded only as a function of time, but Schroedter’s technique minimizes the effect of rate variations on the layer termination process.

3. Level Cut Monitoring

Figure 1 illustrates LC monitoring in its first layer. The layer is terminated when the optical monitor signal reaches a specified photometric level of reflectance (R) or transmittance (T). If the photometric signal is accurate and the index of refraction is as expected from the design, the accuracy would then be only limited by the noise or signal-to-noise ratio (SNR). LC can be precise when done where the slope of the change in %T (or %R) with thickness is great, but it is highly vulnerable to errors in index of refraction and photometric calibration [5]. These two types of error cause the monitor curve to be displaced vertically and thereby cause errors in the LC.

Figure 2 illustrates LC with the optical monitor noise at ±0.2% and terminated at 3 percent of excursion (PE) of the photometric signal change from the last extrema as compared to the photometric difference between the last maxima and minima (or vice versa). It shows the strong systematic errors in the PT of the termination due to index and photometric errors, which could amount to as much as 5 or 10 nm when the index varies from 2.30 to 2.36 and the photometric scale is in error by ±1.0%.

The standard deviation due to noise is small. However, when the PE is small (3%), and the index is lower than expected (2.30), and photometric scale is compressed (to 99% in this case), then the expected termination level is above the level that would be reached by the monitor signal. In such a case, the termination fails entirely. The effects are worse near TP's where the change in %R or %T are small with respect to thickness change. Therefore, the LC approach is the only one discussed here that is particularly sensitive to index and photometric errors, and it would therefore tend to be less favored than the other approaches.

4. Turning Point Monitoring

Figure 1 also shows where the two types of TP determinations can be made at the maxima and minima (extrema), and also where the POEM terminations would be made at a specified percentage of the reflectance excursion between the previous two extrema.

The TP strategy and TP + PT strategy are dependent upon finding the physical thickness at the TP by its shape, which is not affected by errors in the index or photometric level. The POEM strategy is similarly unaffected because it works only with percentages of the distance between extrema, which are not significantly altered by index and photometric errors. The TP’s do not need to be found for POEM; it is only necessary to keep a temporary record of the maximum and minimum photometric values reached in the vicinity of the extrema. The accuracy would again be limited principally by the SNR.

The emphasis in this study is on the POEM strategy [5] and TP strategies. The performances of these are illustrated by examples with a NBP filter and a four-layer broadband antireflection coating (BBAR), but it also will be seen that the judicious use of QCM for thin layers and some other layers at certain monitoring wavelengths also can be expedient.
There are several ways to find a TP when it occurs in an optical monitoring signal. Some of these methods have been described in the earlier paper [5]. The effects of noise in the optical monitor signal are usually the primary cause of layer termination errors. Figure 3 illustrates a typical raw optical monitor signal with ±0.3% noise around a TP at a level of ~31.6%. The choice of layer termination technique will determine how much this noise will cause errors in the accuracy and precision of the layer thickness. The report on another monitoring system [2] stated: “experience seems to indicate that the typical real world photometric noise may be as little as 0.1%, it is usually less than 0.5%, and it rarely is worse than 0.9%.” That paper referred to peak-to-peak noise, whereas this paper uses ±Y% noise, which is twice as large. As a result, this paper would compare at 0.05%, 0.25%, and 0.45%, respectively, with the 0.1%, 0.5%, and 0.9% of the previous paper.

The SNR will depend on the wavelength and %T (or %R) of the monitor signal because of the light source power, optics transmittance, and detector response at that wavelength. One goal of this work is to select the monitoring wavelength that best serves the project at hand. When practical, monitoring all layers at the same wavelength allows the maximum benefit of the principle of monitoring error compensation at the monitoring wavelength, which is most often illustrated in NBP filters. It, however, can also function in many other types of designs.

The “normal” mode mentioned in [2] is similar to the five-point TP detector used here, and the “fitter” mode there is thought to be related to what has been used in this work and referred to as a parabolic fit (P-Fit). Figure 4 illustrates the five-point method. The slope toward a peak or valley is determined at the start of monitoring a given layer by the photometric difference between the first and fifth point. A TP is indicated in a trend toward a peak when the most recent point monitored (#i) is lower than the value of the second previous point (#i-2) (or higher than the minimum in a trend toward a valley). It is probably the simplest and fastest possible algorithm. The software [2] also includes the option to use 3, 5, or 7 points in the algorithm. The greater the noise, the more likely a TP detection will happen before the real TP is reached.

The concept of using a least squares fit of the monitor signal to find a TP has been considered, as was done by Schroedter [4], and is also available in the software of the [2] report. In the latter case, it was found to slow the process sufficiently to be undesirable. Although modern computers are fast, it is still desirable to use the most efficient algorithm, which provides an adequate result and allows the process to run faster for production efficiency.

The “P-Fit” strategy fits the sampled monitor signal points to a parabola as new points are added to the available data, and it predicts where the TP will be in advance of actually reaching that TP. Figure 5 shows that a parabolic curve can be made to fit a sine curve in the region around a TP. The parabola is defined by $Y = a(X - b)^2 + c$, where a defines the curvature at the vertex and b and c are the offsets of the vertex in the X and Y directions.

In the absence of any noise in the data points, three data points in X, Y will define the a, b, and c of the parabola exactly. The problem in this work has been...
to find the best estimate of the position of the TP on the X axis in the presence of various amounts of noise in the optical monitoring signal (Y axis) with a minimum amount of computation time for potential deposition process speed.

In the presence of some noise, if three data points are taken in a close grouping in X at some great distance before the TP is reached, as seen in Fig. 6, the predicted TP is likely to be greatly in error from that of the true TP position in X. If, on the other hand, the three points are widely spaced and cover a range in X that is close to the TP, the prediction will be more accurate. In the optical monitoring case, the points must not extend beyond the TP, since the TP is to be found before or by the time that it is reached. However, it has been found that reasonable predictions for the position of the TP can be determined from data points somewhat before the TP with the P-Fit method, as seen in Fig. 7.

In these simulations, the interval between data points has been taken as 0.2 nm (2 Å), which provides a few hundred data points per quarter wave optical thickness (QWOT) in the visible spectrum. For example, if a QWOT at 550 nm were being deposited at 4 Å per second, that layer would require approximately 2.5 min to deposit. This implies sampling at two samples per second, which is well within the capabilities of current monitoring systems.

This algorithm first filters the optical monitor signal with a moving average of 25 data points. This amount of filtering causes a phase delay of approximately 12.5 points with respect to when the TP is detected. If a 100-point moving average were used, the phase delay would be ~50 points.

The search for the TP in the filtered signal starts at 50 points in physical thickness (10 nm in this case) before the nominal PT where the TP is expected to be found on the basis of the design. The X, Y values of the next three points are used to calculate the predicted TP. It would be correct in the absence of noise, but probably would be highly in error in proportion to any noise.

At the start, the “wheelbase” in X from the first to the third point is only two intervals of 0.2 nm. As new data points are added from the monitoring signal, the first X, Y point is kept the same, but the third point advances with each new point, and the second point used is the point halfway between the first and the most recent data point. Thus, the wheelbase and the stability continues to increase with each new point, and the prediction becomes more accurate until the current PT equals the predicted thickness at the TP (minus the phase factor of 12.5 points in this case).

Figure 7 shows three runs with a noise of ±0.1% full scale of the predicted TP with each new data point. It becomes more accurate with each new point. This algorithm is computationally fast compared to a least squares fit of the data. A line with zero noise is included on the plot for reference, and a straight line also shows the X value or monitor point count of the current point in the search process. When the current X point is equal to the predicted X point, the TP has been found and the search is terminated.

The point to cut in Fig. 7 is seen to be 54.7 ± 0.3 vertically, less the 12.5 points phase offset. Since each point is an increment of 0.2 nm, it implies an error of about ±0.06 nm (or ±0.6 Å) in the TP prediction.

Having found the TP as described above, its associated PT is known from the QCM reading. The addition to this approach, which has been simulated here, is to allow the termination of a layer some physical thickness beyond the TP by adding a specified PT, which is referred to as TP + PT monitoring strategy. The PT in nanometers can easily be calculated from the design in preparation for the actual monitoring. It could be further enhanced by using the data of the QCM at the TP to calibrate the QCM with respect to the optical thickness, and then recalculate the termination point in QCM units. Any error contribution in the PT from the QCM has been assumed to be negligible compared to other errors in
these cases. This extended approach (TP + PT) can be applied to either of the P-Fit or the five-point termination methods after the TP is found.

5. Percent of Optical Extrema Monitoring
As mentioned earlier, the POEM strategy is to terminate a layer at a specified %T (or %R) of the photometric difference between the previous two extrema (maximum and minimum) up or down from the last extrema. The extrema do not need to be in the same layer. This strategy is insensitive to errors in index of refraction or photometric scale, and makes the terminations where the rate of change of %T (or %R) with thickness is large and thereby more precise in thickness determination.

Figure 1 illustrates the POEM technique when monitored at 380 nm. The second layer is terminated at 15.28% of the photometric distance between the last minimum and maximum down from the maximum. The third layer is cut 61.29% up, and the forth layer is cut at 10.04% up after the latest extremum.

6. Termination Point Simulation
The influence of noise and PE (distance from TP) on the PT errors and standard deviation of errors for the termination approaches: POEM, P-Fit, five-point, and LC was reviewed in [5]. Figures 8 and 9 show the results where the noise is simulated at ±0.1, but the index and photometric errors have been kept at zero. In cases of TP terminations, PT has been added after the TP has been found to bring the design to the intended PE level. As Fig. 8 shows, the POEM and LC methods must have a PE greater than ~6% down or up from the extremum to be comparable to the TP detection methods in PT error. Figure 9 shows the standard deviation of errors for the same cases as Fig. 8; the P-Fit is seen to be the best in the range from 0% to 7% PE, while POEM is generally best from 7% PE to higher values.

7. Simulation Examples
The first example shown in Figs. 10–12 is a NBP filter whose design is Glass (1H 1L)3 2H (1L 1H)3 Air, and the substrate in all of these cases has an index of refraction of 1.52, while H is 2.35, and L
is 1.46. In such a classical design, the ratio of the optical thickness of a layer pair (1H 1L) to the thinnest layer in the pair is $2:1$. If the design had layer pairs of (0.667H 1.333L), the ratio would be $3:1$.

The standard 2:1 type above, which terminates each layer at TPs, can be converted to a 3:1 or greater ratio where all of the termination points are at a specified PE from the last extremum. The monitoring wavelength is maintained at the center of the pass band in all cases. Figures 10(a)–10(c) show the progression of this optical thickness adjustment. Figure 10(a) is the common/regular monitor curve at the passband wavelength for the 2:1 design. Figure 10(b) shows the design changed to 3:1 where the cuts are after the TPs, (0.67H 1.33L)3 1.634H (1.33L 0.67H)3. In Fig. 10(c), the design thicknesses have been further adjusted so that all of the even layers are terminated at a PE of 15% from the previous extremum. The resulting design still has the same narrow pass band as the 2:1 design, but tends to widen with increased ratio and PE. If a few more layers are added, it can be made narrower. The adjusted designs also have a somewhat narrower, less dense blocking band. To increase the density, add more layers. Since additional blocking filters are required for most NBP filters, the narrower blocking bands are easily accommodated.

Figures 11(a)–11(c) show the results of NBP filters of the type in Fig. 10(c) with ±0.7% noise in the optical monitor (OM) signal where the cut points are 5%, 10%, and 15% from the extremum. Because 5% POEM is closer to the TP where the slope is less, it shows more effects of the noise. The 2:1 design ratio was used for Figs. 11(d) and 11(e), where

Fig. 11. (a) POEM where the cut point is 5% down from that last extremum in designs of the type in Fig. 10(c); (b), (c) similar to (a) except for 10% and 15% from the extrema; (d) P-Fit strategy to detect a TP; and (e) five-point method.

Fig. 12. (a)–(e) Similar to Figs. 11(a)–11(e) on a narrower band with ±0.7% noise in the OM signal.
PT = 0 in the TP + PT strategy. The design ratio in Figs. 11(a)–11(c) were adjusted as needed to give the required POEM values for each layer-pair. A total of 10% and 15% POEM show more resistance to noise, and in fact this (plus Fig. 8) points to the possibility that a greater percentage of POEM might only be moving toward some point of diminishing returns well before the limit of practical POEM at about 50%.

The TP strategy examples in Figs. 11(d) and 11(e) show the inferiority of the TP finders where the slope at the TP is zero. The TP in these cases is found only by its shape; however, that fact does make it impervious to index and photometric errors.

The five-point strategy has a further problem: it will indicate that a TP has been reached too early, due to the effects of noise and decreasing slope as the TP is approached. This shortfall increases with noise. Figure 11(e) shows the mean peak position to be shifted to shorter than the design wavelength. Figures 12(a)–12(e) show the same cases as Fig. 11, but expand the view around the NBP range. The shift in the five-point case shown in Fig. 12(c) is seen more clearly. The precision of the POEM in Figs. 12(b) and 12(c) can be seen. Figures 12(a)–12(c) are consistent with the previous report [5] that POEM should be greater than 5% to give better precision than TP strategies. Here, 10% and 15% are clearly more precise.

Reference [5] deals with the application of this conclusion to a four-layer broadband (BBAR) design and the choice of wavelength and monitoring type. This BBAR, whose design in nanometers of PT is 12.4356H 34.8891L 118.3713H 88.2478L, is used as the second simulation example. The four-layer BBAR coating design used here has been optimized for the photopic response of the eye, and has been studied by monitoring it at wavelengths from 380 to 800 nm in increments of 70 nm. The monitoring was done initially using only the POEM algorithm (and LC) at a single wavelength and on a single monitoring chip/piece to gain the maximum benefit of error compensations. This approach worked well when monitoring between 380 and 450 nm, but not well at longer wavelengths until between about 660–800 nm was reached. The intermediate wavelengths are not practical with only POEM, primarily because one or more of the terminations are too near a TP. It will be shown that the use of TP monitoring strategies for such layers (and QCM terminations in some cases) can make essentially the whole range from 380 to 800 nm practical for this design.

Figure 13 shows the calculated monitoring curve for 380 nm where the terminations of layers two, three, and four are all well beyond TPs. In such cases, noise does not tend to cause a control breakdown (BD) where the software does not terminate the layer at all. The first layer is terminated at a LC of a specific %R (plus the effects of noise) or by a QCM. In the simple LC termination, the termination levels of %R (or %T) are calculated based on the calibration by the measured %R at the start point for the monitor glass of known index.

Figure 13 also plots the simulated optical monitor signal for this four-layer BBAR at each of the wavelengths studied from 380 to 800 nm. At 660, 730, and 800 nm, only the third layer has a TP before the termination, and thereby offers a good opportunity for a POEM termination of layer three. Other wavelengths have various intermediate situations.

Figure 14 shows the target design plus the results of 10 simulated runs, each with random noise at the wavelengths from 380 to 800 nm, separated by 70 nm. For some percent of full-scale noise at each monitoring wavelength, there is a point beyond which there is a BD where the monitoring does not terminate the layer. This percent noise tolerated before a BD is reached is indicated at the right in the label on each simulation. These are the extreme cases for monitoring at each wavelength. The type of
monitoring for each layer is indicated on each case in Fig. 14 by codes, such as 4111 and 4413. The code is:
1 for a POEM layer cut, 2 for a TP strategy cut of the P-Fit type, 3 for a TP strategy cut of the five-point type, and 4 for a QCM terminations.

Figure 14 shows the best results that could be obtained in this work by searching through the strategy options for each of the four layers at the given wavelength. In all cases, for layer one, the QCM at 4% random error was less sensitive than optical monitoring using a LC. LC monitoring was not used in this work other than examining its use for layer one, because it was shown to be vulnerable to index and photometric scale errors. Except for the cases of this design at 380 and 450 nm, layer two was found best by QCM, strategy 4. Layer three was best terminated by POEM in all cases except at 520 and 590 nm. The TP strategy of the P-Fit type works well for layer three between 520 and 590 nm.

The use of the POEM termination in layer three of this design seems to compensate well for any errors in layer thickness that occur before that point. This is evidenced by the fact that all of the monitoring results in Fig. 14 show little sensitivity to relatively high noise levels. The 380 nm example in Fig. 14 with three layers cut by POEM (i.e., 4111), shows the greatest tolerance for noise (2%).

It is interesting that the best choice for monitoring the fourth layer at wavelengths 660, 730, and 800 nm was the five-point TP strategy. This method tends to cut short in the presence of noise, and under the circumstances, Fig. 13 shows that the fourth layer does not reach a TP as designed for those wavelengths. At 450 nm, the P-Fit worked best because Fig. 13 shows it to have a TP at the end of layer four.

8. Conclusions
This work illustrates how to choose a monitoring wavelength and strategy that offers the best results under the circumstances at hand, based on realistic simulation of the several monitoring strategies. The POEM strategy has been shown to be the most robust when it can be used for 5% PE to greater values. The two TP strategies can be employed, if necessary, and QCM can be used as needed. QCM, however, cannot contribute to error compensation.

The two different TP + PT strategies have been shown to be good choices for terminations that are 7% PE or less. The P-Fit versus the five-point strategy has less systematic error at both low and higher SNR. The photometric level (LC) termination strategy suffers from sensitivity to index and photometric errors, but the other three strategies are essentially insensitive to these errors.

References
3. FilmStar Design from FTG Software Associates, P. O. Box 579, Princeton, New Jersey 08542.