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Strategies for *in-situ* thin film filter monitoring with a broadband spectrometer

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Abstract: Optical monitoring of thin film interference filters is of primary importance for two main reasons: possible error compensation and greater thickness accuracy of the deposited layers compared to non-optical methods. For many designs, the latter reason is the most crucial, because for complex designs with a large number of layers, several witness glasses are used for monitoring and error compensation with a classical monitoring approach is no longer possible for the whole filter. One optical monitoring technique that seems to maintain some form of error compensation, even when changing witness glass, is broadband optical monitoring, as it is possible to record the determined thicknesses as the layers are deposited and re-refine the target curves for remaining layers or recalculate the thicknesses of remaining layers. In addition, this method, if used properly, can, in some cases, provide greater accuracy for the thickness of deposited layers than monochromatic monitoring. In this paper, we discuss the process of determining a strategy for broadband monitoring with the goal of minimizing thickness errors for each layer of a given thin film design.

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1. Introduction

There are several well-established thin film filters monitoring methods available today. If the design (material properties of the thin film layers) and the deposition method allows it, optical monitoring methods are the go-to monitoring techniques. Optical monitoring is often related to error compensation [1,2] and in many cases, the achievable thickness accuracy is superior to non-optical methods [3]. It is therefore not surprising that interest in broadband optical monitoring has remained high for several decades [4–6]. The developments of detectors and the increased computing power of standard computers has increased the accessibility of imaging CCD/CMOS broadband spectrometers. Nowadays, commercially available units are common in the product catalogs of most thin film deposition equipment suppliers.

The advantage of real time spectral measurement is arguably the ability to determine thickness online, which allows for re-optimization of the remaining thin film stack [7,8]. In addition, at least for simple thin film designs, there is no need for a monitoring strategy [8]. These advantages make broadband measurement systems very attractive. In addition, when it comes to determining the strategy, broadband systems offer a greater degree of freedom, as most systems allow for a combination of broadband, monochromatic and rate, or time, or quartz monitoring in the same production run.

In this paper, we will discuss the need for a monitoring strategy if the broadband spectrometer is used for thickness control of complex thin film filters. We will describe the two different methods that use broadband spectral measurement that are available at Institut Fresnel for thin film thickness control. In general, the thought process behind determining the broadband monitoring strategy is very similar to that already published for the automated determination of the monochromatic strategy [9]. The difference is that, instead of changing the wavelength, the wavelength range is adapted for each of the layers if necessary. Non-optical monitoring methods

are frequently used for a given layer if the possible thickness error is smaller than that of optical methods. We experimentally demonstrate broadband monitoring strategies on several thin film filters with increasing complexity.

2. Experimental setup

The deposition of the filters was performed with the HELIOS 400 and HELIOS 800 plasma-assisted reactive magnetron sputter deposition (PARMS) machines developed by Bühler Leybold Optics [10]. The in-situ measurement of the thin film was performed with the WB-OMS developed by Bühler Leybold Optics, consisting of the WBM-1000 spectrophotometer and the deposition control software – TOMS.

For experiments described below, transmittance measurements were performed. The WBM-100 uses a standard halogen lamp as a light source. A collimating lens is placed at the focal distance from the lamp to collimate the part of it that is sent through the sample. Light is then collected into an optical fiber using another collimating lens and this fiber is directly connected to the spectrometer. The usable wavelength range for these experiments were set to 400-900 nm in order to secure highest signal to noise ratio. However, the spectrometer can support measurements from 350-1200 nm.

The TOMS software, also developed by Bühler, analyzes the spectral measurement and determines when the deposition has to be stopped. The software allows to use broadband, monochromatic and rate monitoring in a single deposition run.

The ex-situ characterization of the filters was performed by a *Lambda 1050* spectrophotometer from PerkinElmer. The designs were calculated with *Optilayer* software, using refractive indices determined by spectrophotometric reverse-engineering with an in-house written program.

3. Method

There are two popular algorithms that are classically used with the broadband measurement – *Merit* and broadband thickness (*Wideband*). The *Merit* algorithms tracks the measured spectrum and compares it to the theoretical one, and the layer deposition is completed when the distance (merit) between the two is minimum [11]. With *Wideband*, the recorded spectrum is used to adjust the value of the deposited thickness after each sequential measurement. From this fitted thickness, the deposition rate is calculated and used to determine the remaining deposition time [12]. An example of these two algorithms is given in Fig. 1 where a 23 nm thick Nb₂O₅ layer deposited on a fused silica substrate is monitored by the broadband *Merit* Fig. 1(a) and the *Wideband* Fig. 1(b) algorithms.

In both of these examples, there is a slight overshoot, and the deposition is completed a little too late. The error in both cases is ~0.1 nm. As can be seen from the measured online deposition rate curves, the deposition rate, determined from online fitting of the broadband measurement, is not stable in the first 10-15 seconds, illustrating the difficulty of the thickness control for the very thin layers.

Similar to monochromatic monitoring where the choice of the control wavelength is crucial, the most important input parameter for broadband monitoring is the wavelength range for the measurement and the processing. This parameter can, and in certain situations, should be, adjusted for each layer. There are several reasons to adjust the wavelength range, related to the technical capabilities of the monitoring setup and the designs themselves.

One area where broadband monitoring systems are inferior to monochromatic systems is spectral resolution. The spectral resolution of the broadband systems is not adjustable and depends primarily on the number of pixels in the sensor. In the case of the broadband monitoring system used in this research (*WBOMS-1000*), the resolution is fixed at 3.5 nm. Therefore, when selecting the wavelength range for monitoring a given layer, it is advantageous to adjust the spectral range to avoid sharp peaks in the spectrum. An example is shown in Fig. 2 where the

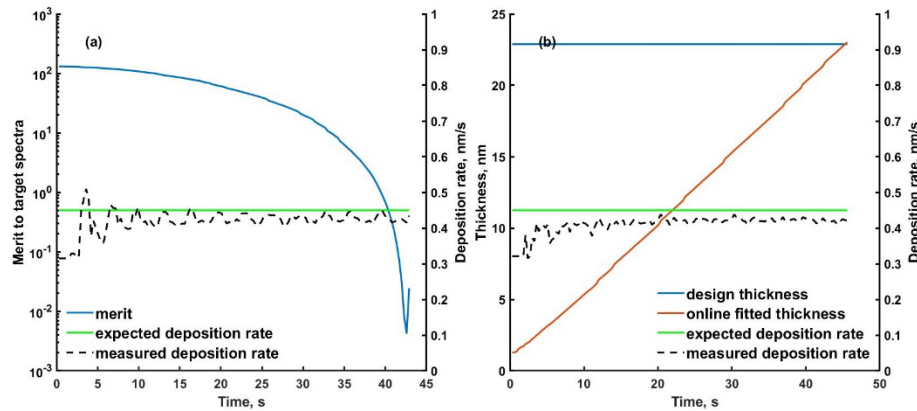


Fig. 1. Example of 23 nm thick Nb₂O₅ layer deposited on a fused silica substrate controlled by broadband Merit (a) and Wideband (b).

theoretical spectrum of the 31st layer from a design inspired by the OIC manufacturing contest is compared to the same spectra when a 4 nm spectral resolution is considered. The challenges of the designs and manufacturing difficulties of the OIC 2022 thin film manufacturing contest will be discussed in detail in the discussion section.

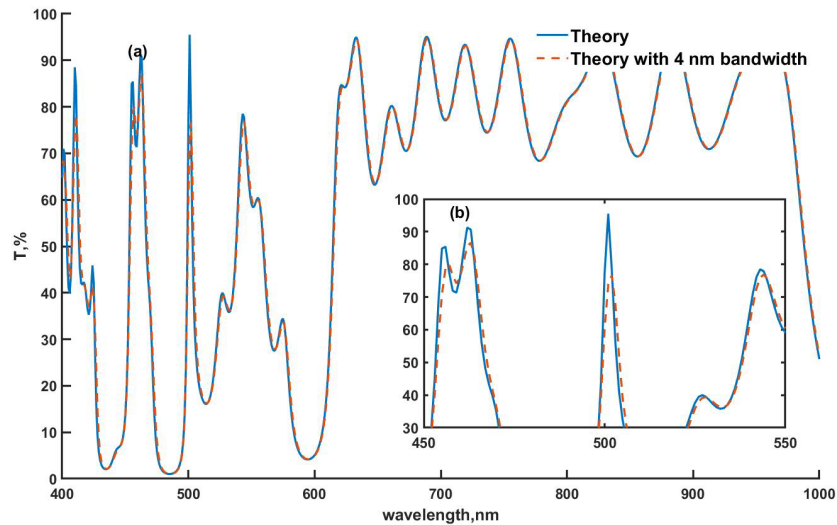


Fig. 2. Example of the limits of spectral resolution. Theoretical spectra of layer 31 from OIC contest filter compared to the theoretical design calculated with 4 nm bandwidth: (a) full scale, (b) zoom in for shorter wavelengths.

As can be seen, the spectra show sharp peaks at the shorter wavelengths, which cannot be matched when considering a spectral resolution of 4 nm. However, the two spectra plotted in Fig. 2(a) overlap in the longer wavelength range (above 600 nm), so, in order to stay as close as possible to the theoretical conditions, the shorter wavelengths must be excluded from the monitoring wavelength range for this particular layer. The monitoring software (TOMS) has a function to adjust the target curves with respect to the spectrophotometer bandwidth – the bandwidth of the setup is included in the target curve calculations. This function works very well if the spectral peaks of the design are relatively wide (~3-4 nm FWHM). However, for very

narrow spectral peaks as in the example in Fig. 2(b) (less than 1 nm FWHM), it is advantageous to adjust the monitoring wavelength range excluding these kinds of spectral peaks to reduce the chances of layer being terminated at wrong thickness. This is probably due to an approximate modeling of the spectral bandwidth of the BBM setup, as it is not exactly known, wavelength by wavelength. Improving the theory-experiment agreement for such spectrally fine peaks would require deeper investigations, wavelength by wavelength.

Another factor to consider when selecting the wavelength range is the maximum variation in transmittance amplitude when depositing the layers. This is particularly important if the first layers of a filter are thin (20-50 nm). For such designs, the transmittance will vary much more in the short wavelength range than in the long wavelength range. Therefore, measurements at longer wavelengths will be more influenced by measurement noise than by increasing layers thickness associated transmittance change.

The amplitude of transmittance can be problematic not only for thin layers at the beginning of a design, but also for relatively thick layers in the case where the admittance of the partially deposited coating is close to the index of the layer under consideration. An example is shown in Fig. 3 where the variation of transmittance with increasing thickness and wavelengths is shown for the 7th layer of Nb₂O₅ (that is nearly 100 nm thick) from an antireflection design described in in the discussions section.

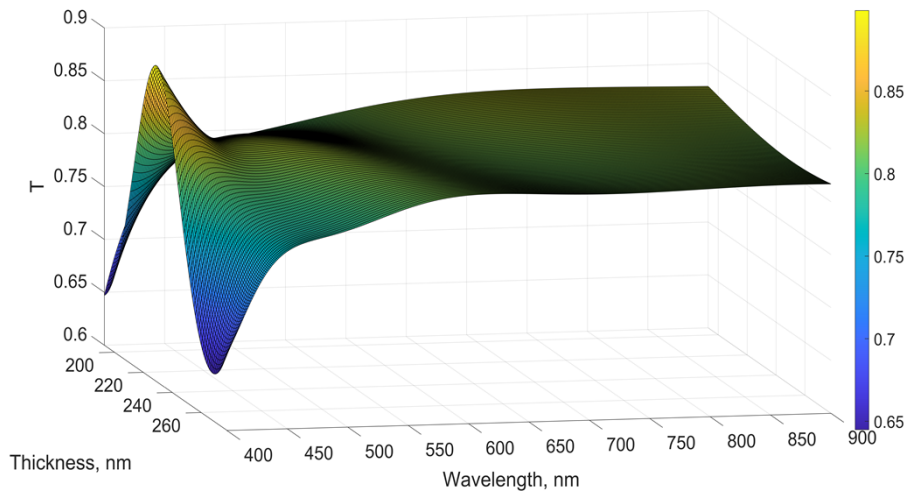


Fig. 3. Example of transmittance amplitude as a function of thickness and wavelength.

As can be seen, the transmittance barely changes for the entire spectral range as thickness increases. Although the change appears significant in the 400 nm wavelength range, these wavelengths cannot be used due to the limitations of spectral resolution (both for broadband or monochromatic monitoring) and the fact that the trigger point is too close to the previous turning point (*swing out* is not sufficient for monochromatic monitoring [13,14]). Therefore, optical monitoring of this layer will result in a larger thickness error compared to non-optical methods such as deposition rate or quartz crystal microbalance monitoring. Preliminary experimental tests of broadband monitoring of these first layers including this spectral ranges with these narrow peaks (using both merit and wideband), resulted in very high (20-30%) thickness errors.

Because of these considerations, broadband monitoring systems cannot be used as *plug and play* units and monitoring strategies must be determined to avoid weaknesses of the monitoring setup and the design.

3.1. Taking into account the measurement of the thickness error of each layer

Currently, the re-optimization of the thin film stack is not implemented in the TOMS software, but it could be done manually by the operator if necessary. Thickness errors however are not ignored, for all experimental runs presented here, the target curves were adjusted for each layer based on the measured thickness errors of the previous layers. Indeed, if we consider a design consisting of n layers with thicknesses $d_1..d_i..d_n$. We can calculate the transmittance $T_i(d_1, d_2, \dots, d_i)$ after the layer i . However, if we know that a thickness error (e) has occurred in the layer $i-1$, we can use this information to calculate a new adjusted transmittance ($T_i(d_1, d_2, \dots, d_{i-1} + e, d_i)$) corresponding to the real deposited stack. By using the adjusted transmittance for the target curves, the thickness errors of the deposited layers are kept low as we eliminate the associated transmission bias for stopping the new layer. However, the target curve for the last layer will no longer match the original design.

4. Results and discussion

The technical and design considerations for broadband optical monitoring are similar to those for monochromatic monitoring, so by slightly adjusting the wavelength selection process for monochromatic monitoring [9], we can create broadband monitoring strategies.

Our current experience suggests that the wavelength range for broadband monitoring can be as low as 50 nm. However, in the case of such a narrow usable wavelength range, we use monochromatic monitoring, as the system allows for a combination of methods.

Layers that cannot be controlled with optical measurement were controlled by rate monitoring. With rate monitoring, the layer is deposited for a certain amount of time, and this time is calculated from the average deposition rate extracted from the previously deposited layers. With the broadband system, the deposition rate is determined from the spectral measurement, the accuracy depends on the precision of the spectral measurement and the thickness fitting method. In contrast, the deposition rate determined from a monochromatic measurement is also sensitive to thickness errors. Therefore, including rate monitoring in the strategy using the broadband measurement system is arguably better than including rate monitoring in the strategy using the monochromatic system. Simply because the in-situ deposition rate estimation is more precise.

Monitoring strategies that include broadband, monochromatic and/or rate monitoring methods will henceforth be referred to as mixed monitoring strategies.

4.1. Antireflective coating

We first considered an antireflection coating consisting in 20 alternated $\text{Nb}_2\text{O}_5/\text{SiO}_2$ layers on fused silica substrate with layers thicknesses ranging from 5 to 145 nm (see [Supplement 1](#) for design details). Such a simple design might appear easy to fabricate; however, several parameters make it a challenging one. Half of the layers in this design cannot be optically monitored. Not only the thinnest but also the thickest layers in this design have to be monitored using rate criterion because of the negligible change in transmittance during deposition in the entire monitoring spectral range. An example was already shown in Fig. 3, where the transmittance of the 7th layer is plotted as a function of thickness and wavelength. Similar shallow surface is observed for 3 other thick layers (layers nr. 12, 17, and 20) in this design.

Therefore, the monitoring strategy for this filter design is a combination of rate and broadband monitoring, where the wavelength range is varied for the layers with the goal of maximizing the transmittance change as layer thickness increases. Rate monitoring is used for the layers where the transmittance change is not sufficient for reliable optical measurement. The strategy and design are shown in Fig. 4. The broadband thickness (*wideband*) algorithm was used to control the thicknesses of the layers that were monitored optically.

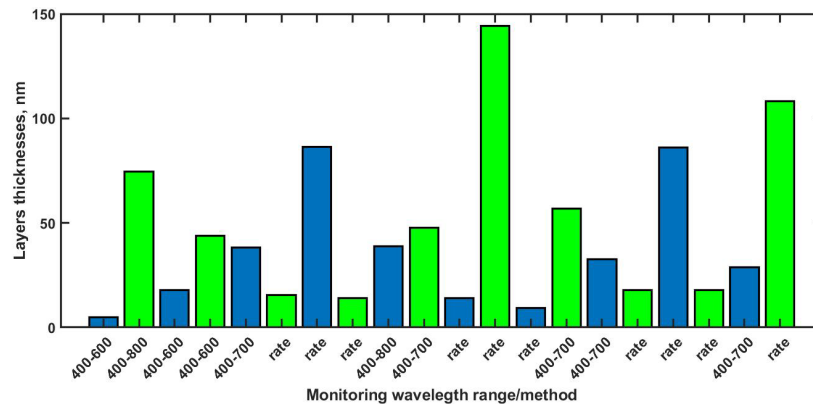


Fig. 4. Layers thicknesses and monitoring strategy for the 20-layer AR design. High index layers are in blue and low index layers are in green.

The transmittance of the deposited filter is shown in Fig. 5. As can be seen, the correspondence between experiment and theory is pretty good, oscillations in the shorter wavelength range are shifted in the y-axes, with a maximum deviation of 0.5%, possibly due to thickness or refractive index errors. However, there is no visible shift in the x-axis. The shift in experimental spectrum at 860 nm is related to the change of detectors in the spectrometer.

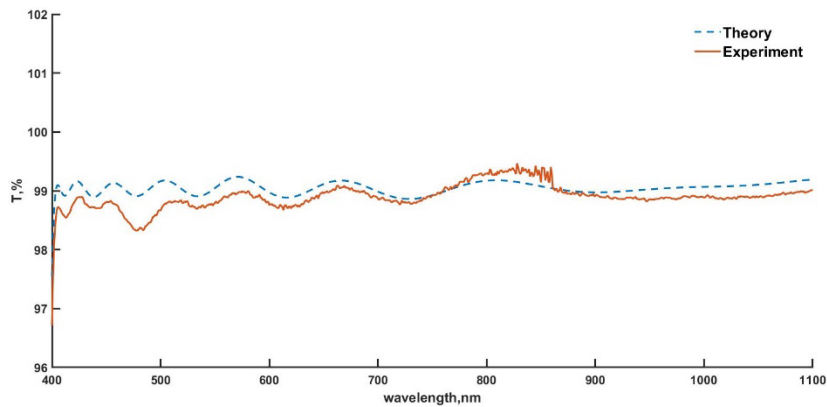


Fig. 5. Theoretical spectra compared to measured spectra of the AR design without backside reflection.

However, since neither broadband nor rate monitoring are known to be error-compensating monitoring methods, the good match between the theory and experiment is the result of very small thickness errors that would correspond to average random thickness errors for each layer of $\sim 0.2\text{-}0.3\%$.

4.2. D65 compensator filter

This design consisting in 37 alternated Nb₂O₅/SiO₂ layers with thicknesses ranging from 10 to 507 nm (see Supplement 1 for design details) is made to ‘flatten’ the power distribution of the CIE D65 illuminate standard [15]. The illumination power distribution, design, and multiplication of the power distribution profile with the theoretical filter are given in Fig. 6. Since we had previously fabricated this filter using the polychromatic strategy (changing the monitoring wavelength for each layer) [9], we were interested in comparing the results with broadband monitoring.

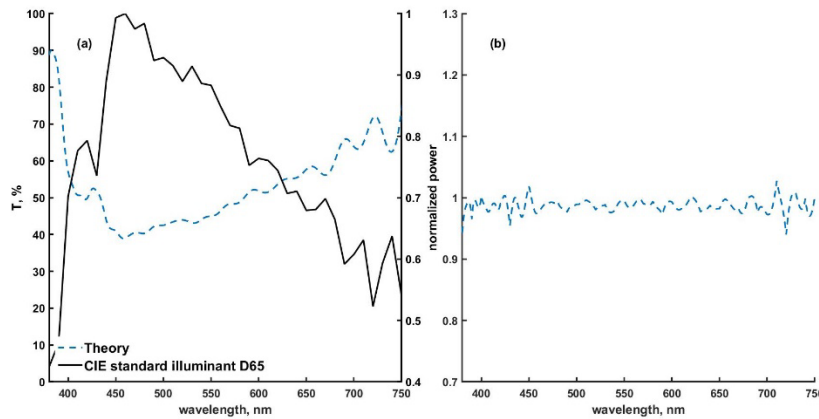


Fig. 6. (a) Power distribution of CIE D65 and theoretical filter spectrum as a function of wavelength; (b) multiplication of power distribution with theoretical filter spectrum.

From design analysis and first simulations, it is clear that all layers of this design cannot be monitored with broadband algorithms and that a mixed strategy is necessary. Since the first layers are either thin or have negligible refractive index contrast (1st layer made of silica deposited on silica substrate), the transmittance change is not sufficient in the wavelength range of interest. Therefore, layers 2, 3 and 4 were set for monochromatic monitoring and layers 1 and 5 – where the transmittance amplitude was not significant even for one wavelength - were rate monitored. The monitoring wavelengths for the layers 2-4 were selected by the previously published polychromatic method [9]. For the remaining layers, the broadband setup could be used as it is, with no need to change the wavelength range. The layers thicknesses and the associated monitoring wavelengths/methods are summarized in Fig. 7.

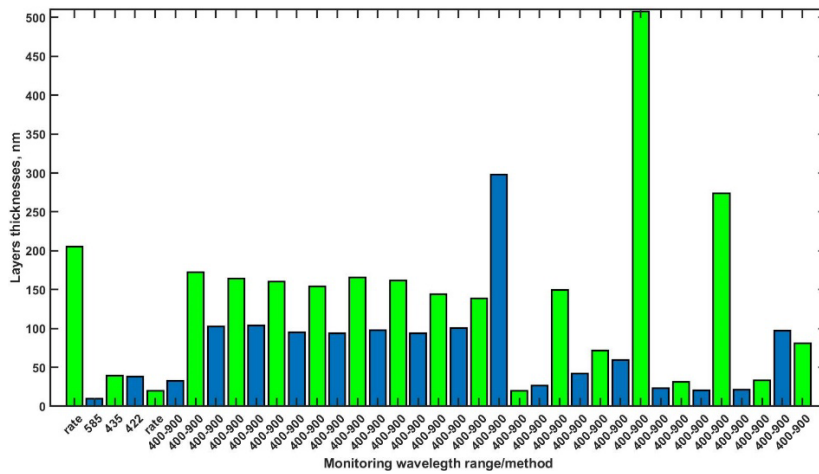


Fig. 7. Layer thicknesses and monitoring strategy for the D65 compensator design. High index layers are in blue and low index layers are in green.

The performances of the obtained filters controlled by broadband and monochromatic systems are presented in Fig. 8. From the multiplication of the obtained filter spectrum with the power distribution of the D65 standard (Fig. 8(b)) it is clear that the performance of the filters obtained

by mixed monitoring strategies with broadband monitoring outperforms the previously obtained filter controlled by a monochromatic monitoring (polychromatic strategy).

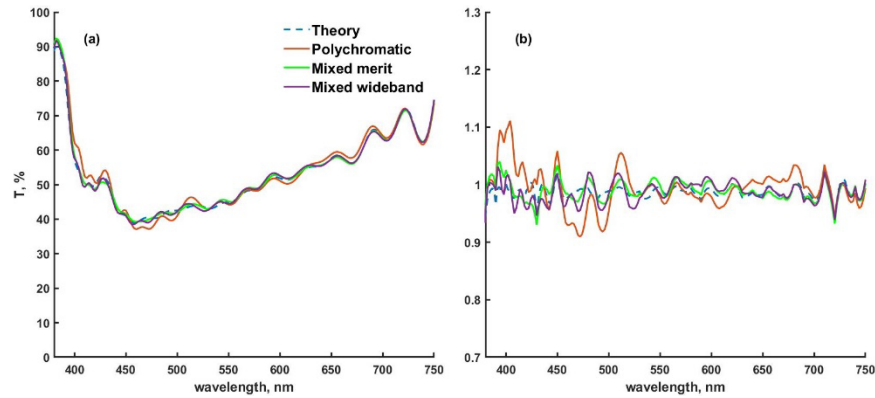


Fig. 8. (a) Theoretical spectra compared to measured spectra of the D65 filter monitored by different strategies; (b) multiplication of measured spectra with the CIE D65 power distribution.

It is hard to distinguish the results obtained with a mixed strategy where *Merit* and broadband thickness (*Wideband*) methods are used as the dominant monitoring method. Looking very closely at the whole process it appears that the *Merit* method has slightly smaller thickness errors. The measured deviations from theoretical performances correspond to average random thickness errors for each layer of $\sim 0.2\text{--}0.3\%$.

4.3. OIC manufacturing contest 2022

2022 OIC manufacturing contest consisted in fabricating a visible/near-IR filter with staircase profile, each step having a one order of magnitude transmission difference [16]. The challenge of this problem relies on the fact that the target design has several very abrupt (vertical) changes in transmittance, which are not easily replicated by thin film structures due to limited achievable spectral frequencies (which generally require quite thick designs). However, our main objective at this stage is to test the broadband spectrometer, we were especially interested in a multi-witness glass strategy, as the previous experiments suggest that thickness errors should be small, if broadband setup is used correctly. Therefore, our first design approach was primarily focused on a realistic filter to fabricate rather than completely matching the OIC target, we opted for a 68-layer solution consisting of alternated $\text{Nb}_2\text{O}_5/\text{SiO}_2$ layers with thicknesses ranging from 20 to 478 nm deposited on N-BK7 glass (see Supplement 1 for design details). Minimum layer thickness of 20 nm was used in order to avoid possible uncertainties linked to unstable deposition rate during the first few nanometers of deposition. The calculated theoretical spectra of the design and performance of the manufactured filter are shown in Fig. 9.

For monitoring the different layers, the broadband system was used again, and a mixed broadband *Merit* and rate monitoring strategy was developed. The wavelength range for the layers monitored with *Merit* was adjusted to avoid sharp features in the spectra and maximize the change in transmittance as the thicknesses of the layer's increases. The design and wavelength ranges are given in Fig. 10. Since the number of layers was relatively high, a two-witness glass strategy was considered, and the new witness was used starting from layer 35 until layer 68. Rate monitoring was used for 7 layers for which a sufficient change in transmittance was not obtained as layers' thickness increased. Insufficient change in transmittance was exclusively a problem for very thin layers, unlike the AR filter. For the other layers, lower limit of the spectral range was adapted to avoid spectral features with high frequencies.

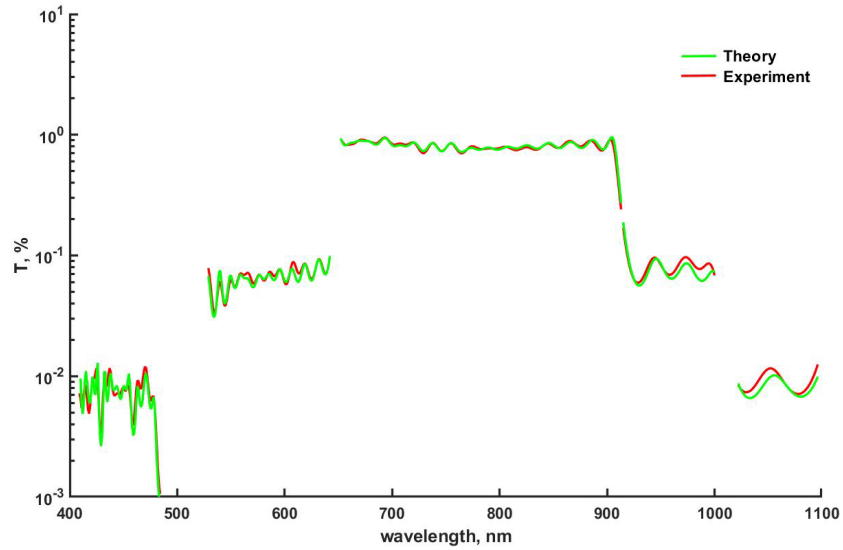


Fig. 9. Designed (in green) and measured (in red) spectral responses of the 68-layer filter presented in logarithmic scale.

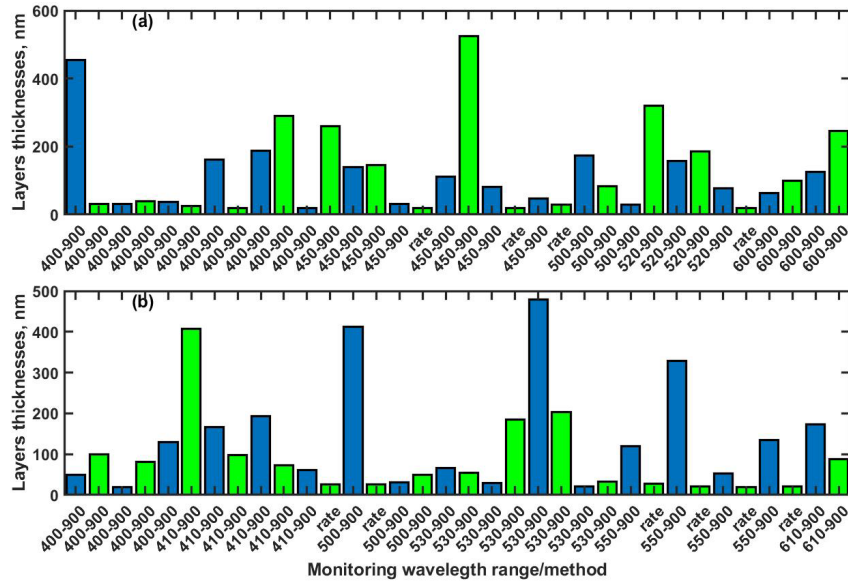


Fig. 10. Layer thicknesses and monitoring strategy of the OIC contest design: (a) glass witness 1, (b) glass witness 2. High index layers are in blue and low index layers are in green.

As can be seen in Fig. 9, the agreement between the designed and the measured spectra is very close. For the design contest, the transition in the 900 nm region should be much sharper to be close to the theoretical target provided by the organizers. To create a design that matches the sharp transition, the total thickness of the coating should be considerably higher increasing the number of layers to be monitored to several hundred. This would of course significantly increase the total deposition time required to make such filter. However, the results plotted in Fig. 9 gives confidence that multi-witness glass strategies for the broadband monitoring system would be a good solution for monitoring of complex thin film filters, as the thickness errors can be kept relatively small. Additional theoretical simulation shows that to obtain a filter of such performance, the random thickness errors for the layers should be below 0.5%.

5. Conclusions

We have tested broadband monitoring on a variety of designs. It is clear from these results that broadband monitoring is not a ‘*plug-and-play*’ solution for optical monitoring and that a monitoring strategy is required for the majority of thin film designs. Multilayer filters with near- theoretical performances can be achieved with the broadband system if the wavelength range is adjusted to maximize the signal amplitude for a given layer and if the spectral resolution limitations are avoided. In addition, the inclusion of other monitoring methods (such as rate and monochromatic monitoring) in the strategy allows for a deposition run with low thickness errors and, therefore, good agreement between theory and experiment can be obtained over the entire spectral range of interest. The small thickness errors of the deposited layers are particularly important for complex designs that cannot be monitored on a single witness glass.

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Data availability. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

Supplemental document. See [Supplement 1](#) for supporting content.

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