Advantages and challenges of optical coating production with indirect monochromatic monitoring

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In this paper, we present our recent studies on raising the quality of optical coating production with an indirect monochromatic monitoring system. Preproduction error analysis and computational manufacturing are used to estimate potential advantages of application of indirect optical monitoring. It is then demonstrated that a key issue for realization of this advantage is accurate specification of tooling factors for layer thicknesses on test glasses. The tooling factors are precalibrated using single layer depositions and then are corrected using results of reverse engineering for the first production run. It is found that a gradual variation of tooling factors of low index layers is the main error factor in the first deposition run. Finally, we redeposit our coating with a modified monitoring strategy, taking into account this factor. The new experimental results show excellent correspondence with the theoretical spectral performance.

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1. Introduction

Demands on optical coatings with sophisticated spectral performances are increasingly growing [1–3]. Reliable monitoring of their production becomes key to success in many application areas [4–6]. There exists a great variety of different monitoring approaches. Optical monitoring that possesses high accuracy of optical thickness control has attracted the interest of many researchers. It can be subdivided into monochromatic monitoring and broadband monitoring techniques. In this paper, we consider optical monitoring that employs monochromatic spectrophotometric measurements.

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A commonly used classification of monitoring techniques subdivides monochromatic monitoring into direct and indirect monitoring. In the case of direct monitoring, transmittance or reflectance measurements are performed on at least one of the coatings to be manufactured. There are many obvious advantages of direct monitoring arrangements, but there is also an essential disadvantage that small errors in early layers affect monitoring of later layers [3], and the cumulative effect of errors can destroy spectral properties entirely. There are theoretical researches on direct monochromatic monitoring systems aimed at eliminating accumulation of thickness errors [7,8], but such systems have not yet been realized.

In this paper, we consider only indirect monochromatic monitoring; layer thicknesses are monitored on separate witness substrates. Turning point monitoring is out of the scope of this paper, and we concentrate our attention on monitoring strategies connected with what is called "level monitoring" [9,10]. This means that a layer deposition is terminated when transmittance or reflectance reaches a certain level different from transmittance or reflectance extreme values. Level monitoring is often used in the form of monitoring by swing values [3,10–13]. This type of monitoring is especially advantageous in the case of optical coatings with thick layers when at least one monitoring signal extremum is registered during layer depositions [3].

The main advantage of the indirect monitoring is to prevent accumulation of thickness errors with the growing number of deposited layers [14,15]. Typically, for optical coatings with a number of layers exceeding 30–40, the strong cumulative effect of errors is observed when direct monitoring is used, while errors are small for the indirect monitoring strategy when separate monitoring chips are used for each pair of H and L layers. At the same time, monitoring of layer thicknesses on separate witness substrates presents a certain disadvantage. The witness chip may be of a different material and at a different temperature as compared to the deposited sample substrate. Errors in the thicknesses of the various layers of the system are uncorrelated, and systematic errors can occur if the calibration is not properly carried out, or if the process parameters depart from those during the calibration run [14]. Therefore, accurate calibration of tooling factors for each material is the main challenge in the indirect monitoring.

In Section 2, we discuss the choice of design that is the most suitable for indirect monitoring by swing values and estimate advantages of this type of monitoring using preproduction error analysis and computational manufacturing experiments. In Section 3, we discuss calibration of tooling factors of the two materials using single layer depositions and consider results of the first test deposition run. In Section 4, we thoroughly analyze possible errors of the deposition process. Reverse engineering of the produced coatings on the basis of off-line transmittance data allows us to perform more accurate analysis of tooling factors. It is found that the tooling factors of the low-index layers vary gradually during the deposition process. In Section 5, the obtained information is used to provide feedback to the deposition process. The results of a new deposition run demonstrate essential improvement of the discrepancy between theoretical and measured data. Final conclusions are presented in Section 6.

2. Advantages of Indirect Monitoring: Preventing the Accumulation of Thickness Errors

We consider a hot mirror (or heat mirror; see [3]) as the example of an optical coating where the advantages of indirect monitoring can be fully realized if the optical coating design is properly chosen. Our hot mirror performance satisfies the following

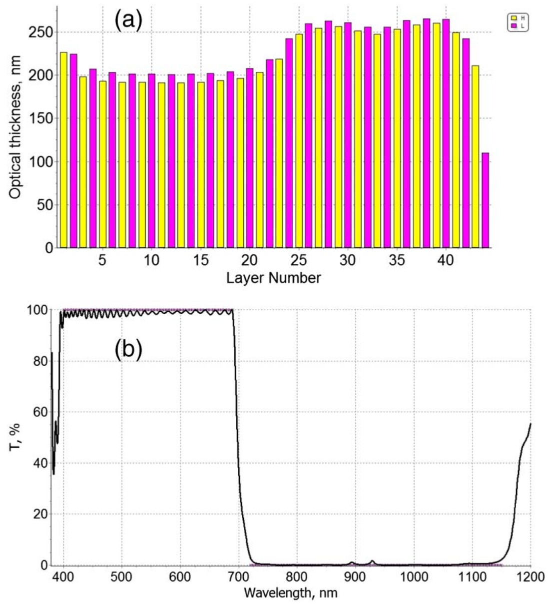

Fig. 1. (a) Layer-thickness profile of an ultrasteep hot mirror obtained by stochastic constrained optimization. (b) Calculated transmittance of the hot mirror.

demands under normal incidence: target transmittance is 100% (no backside reflections included) in the wavelength range of 400–690 nm, and target transmittance is 0% in the spectral region from 720 to 1150 nm (target transmittance is shown by the purple dots in Fig. 1). In the design process, we use Ta_2O_5 and SiO_2 as the high- and low-index materials, respectively. The substrate is B270 glass of 1.5 mm thickness, and the incident medium is air.

As mentioned previously, we consider the indirect level monitoring in the form of monitoring by swing values. A swing at the end of layer deposition (the final swing) is defined as a ratio of two special values calculated based on the monitoring signal (backside reflectance in our case). The first value is the difference between signal termination level and preceding signal extremum, and the second value is the difference between signal extrema. The main advantage of the monitoring by swing values is that neither scaling calibration errors nor signal drifts for constant values influence the final swing values. But this advantage can be realized only if coating layers are thick enough and at least one signal extremum can be traced during each layer deposition.

For designing of the hot mirror without thin layers, we applied the stochastic constrained optimization [16,17]. The lower and upper constraints for layer optical thicknesses were 100 and 350 nm. The layer thicknesses and spectral response of the final design are shown in Fig. 1. The average transmittance is higher than 98% in the pass spectral region, and the reflectance is higher than 99% in the wavelength region of 720–1150 nm. The main structure of the final design can be interpreted as two short-wave-pass eighth-wave/quarter-wave/eighth-wave stacks with the central rejection wavelength of about 830 and

1040 nm. The H L/2 layer pair is inserted between the substrate and the stack as a broadband antireflection (AR) coating to reduce oscillations in the passband [18]. The obtained design has no thin layers and is suitable for accurate monitoring during the deposition (Fig. 1).

To estimate a potential advantage of the indirect monitoring, we perform a preproduction error analysis for three different monitoring strategies. Monitoring Strategies 1 and 2 are direct monitoring strategies; the first is based on the choice of the most sensitive wavelength [13,19], while the second, proposed in [8], is specifically developed for minimizing the cumulative effect of thickness errors. Monitoring Strategy 3 is the indirect monitoring using separate monitoring chips for the each pair of H/L layers. For specifications of this strategy, i.e., for choosing monitoring wavelengths for each pair of layers, a new monitoring option of OptiLayer software [16] is applied in order to select the minimum number of different monitoring wavelengths providing final swing values in the ranges from 20% to 70%.

For the preproduction estimation of errors in layer thicknesses [7], we simulated random errors in the measurement data; in all experiments, these errors were distributed by the normal law with zero mathematical expectation and standard deviation equal to 0.1%. It is referred to as the level of errors in measurement data.

Figure 2 presents the expected levels of errors in the thicknesses of layers of the hot mirror. Strong accumulation of errors with the growing number of deposited layers is observed when optical monitoring Strategy 1 is used. In the case of the monitoring Strategy 2, the accumulation of thickness errors is still observable, and thickness errors of about 2% and more are expected for many layers. Strategy 3 provides the smallest level of errors, all of them are less than 1%, which proposes a significant advantage over Strategies 1 and 2 for the specific coating under consideration. Below, we show that this conclusion is confirmed by the results of computational manufacturing experiments.

In the course of computational manufacturing experiments, major factors causing production errors in the real deposition chamber were simulated [20]. The mean rate of the high-index material was 0.3 nm/s, and root mean square (rms) rate fluctuation was 0.015 nm/s; for the low-index material these parameters were 0.8 nm/s and 0.06 nm/s, respectively. Mean shutter delays were taken equal to 350 ms, and rms deviations of the shutter delay were 100 ms. We simulated random errors having approximately 1% noise level in the measurement data.

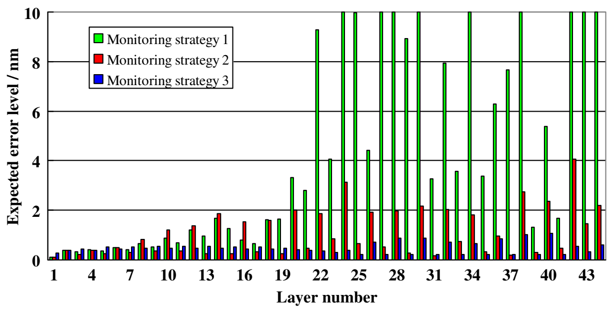

Fig. 2. Expected levels of errors in the thicknesses of layers of the hot mirror with different monitoring strategies.

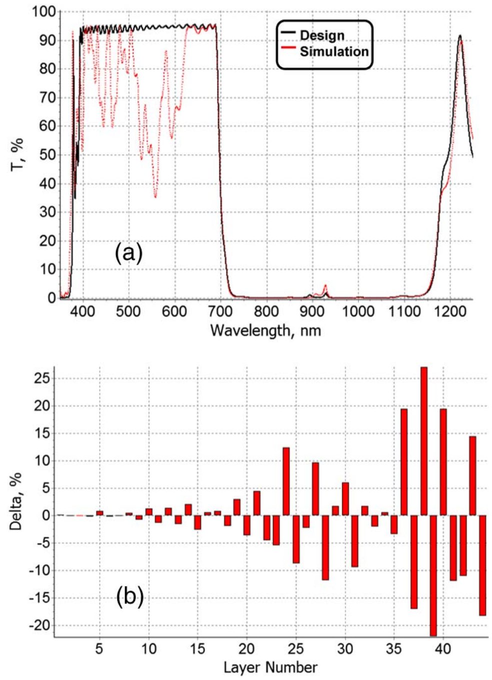

Fig. 3. (a) Theoretical transmittance of the hot mirror (dark curve) and transmittance of the computationally manufactured coating (red curve). (b) Typical errors in layer physical thicknesses.

We performed 50 computational manufacturing runs with the three monitoring strategies. In the first case, all runs were unsuccessful, the monitoring Strategy 2 exhibited a production yield of about 30%, and all 50 runs were successful in the case of Strategy 3. We considered a computational run as successful when the transmittance of the manufactured coating deviated from the target transmittance for less than 5% in the operational spectral regions. In Fig. 3, we show results of the best run of Strategy 1; one can see that, even in the case of this run, the strong cumulative effect of errors after depositing 20–25 layers destroys hot mirror spectral performance entirely.

The cumulative effect of thickness errors was much less in the case of the monitoring Strategy 2; nevertheless, it was still too high for reliable manufacturing of the hot mirror. Plots of transmittance and errors in layer thicknesses for the computationally manufactured coatings are not presented here.

In contrast with monitoring Strategies 1 and 2, Strategy 3 enables full elimination of the effect of accumulation of thickness errors, as shown in Fig. 4. Transmittances of manufactured mirrors (solid curve) deviate from the theoretical transmittance (dashed curve) for not more than 2%. The typical

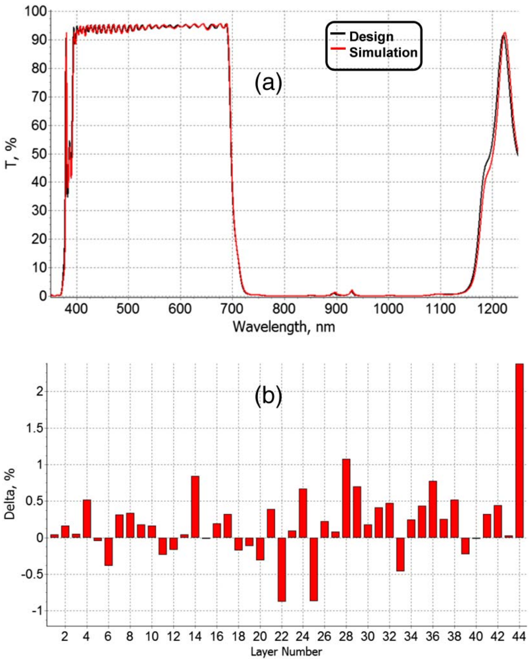

Fig. 4. (a) Theoretical transmittance of the hot mirror (dark curve) and transmittance of the computationally manufactured coating (red curve). (b) Typical errors in layer physical thicknesses.

distribution of layer thickness errors is presented for one of the computationally manufactured coatings. One can see that there is no accumulation of thickness errors during the coating deposition, and the level of errors is less than 1%.

Thus, using indirect monitoring with several monitoring chips instead of just one can prevent the accumulation of errors for the hot mirror in the monochromatic monitoring system.

3. Precalibration of Tooling Factors and Results of the First Coating Run

As mentioned above in the case of the indirect optical monitoring technique, the main challenge is the accurate calibration of tooling factors presenting the ratios of thicknesses on witness chips and substrate. This calibration was done by preproduction depositions of single Ta_2O_5 and SiO_2.

For the coating production, we used the Optorun electron-beam deposition plant. During the deposition, layers were densified with an RF-type ion source. Thereby, the selected deposition parameters resulted in coatings without any relevant shift after cooling and venting. The indirect monochromatic backreflection optical monitor was utilized to control thicknesses of deposited layers. Quartz crystal monitoring was performed in parallel and mainly used as feedback for stabilizing evaporation rates [21].

After the deposition, the refractive indices and thicknesses were derived from the spectral responses of the produced samples using OptiChar software [16]. Thicknesses of the films on the monitor glasses were derived from the swing level, and the ratios of the above thicknesses were used to define tooling factors. This gave tooling factors equal to 0.973 and 0.916 for Ta_2O_5 and SiO_2 layers, respectively. These values are in remarkable correspondence with the values reported in [21].

Table 1. Wavelength Dependence of Refractive Index of Ta_2O_5 and SiO_2 Films Found in the Frame of Homogeneous Thin Film Model

Wavelength/nm	SiO_2	Ta_2O_5
400	1.4823	2.3073
500	1.4724	2.2302
600	1.467	2.1928
700	1.4638	2.1718
800	1.4617	2.1588
900	1.4602	2.1502
1000	1.4592	2.1441
1100	1.4584	2.1397
1200	1.4579	2.1364

Table 1 presents wavelength dependencies of the refractive indices of the Ta_2O_5 and SiO_2 films. They are shifted upward from the previously used in [21] dependencies for approximately 0.01 and 0.005, respectively; it is rather small and can be connected with systematic errors in reflectance data. Therefore, the refractive indices in our deposition technique are quite reproducible from run to run.

According to the preproduction analysis in Section 2, for the hot mirror deposition we applied the monitoring strategy in which one monitoring chip is used to control thicknesses of two subsequent high- and low-index layers. The sequence of monitoring wavelengths was shown in [22]. After the first deposition run, the transmittance of the sample was measured at normal incidence in the spectral range from 350 to 1200 nm using a Cary5000 spectrophotometer. The measured transmittance of the hot mirror is depicted in Fig. 5, where the theoretical transmittance calculated by taking into account the backside reflectance from the B270 substrate is also presented. In this figure, good agreement between theoretical and experimental data is observed. However, there is still observable discrepancy between two transmittance curves, especially in the 1150–1200 nm range. This indicates the presence of errors in layer parameters.

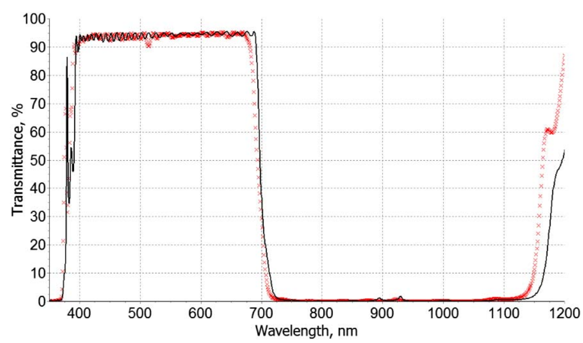

Fig. 5. Comparison of measured transmittance data (red crosses) and theoretical transmittance (solid black curve) of the hot mirror.

We reveal the origin of these errors in the next section.

4. Error Analysis and Reverse Engineering for Accurate Determination of Tooling Factors

As mentioned above, there are inconsistencies between experimental and theoretical transmittance data. In the deposition process, all major factors affecting the deposition process and causing errors in layer parameters can be divided into three parts: variation of optical constants, variation of film thicknesses caused by optical monitoring, and variation of tooling factors. In this section, we perform full error analysis and reverse engineering in order to find possible reasons for the observed deviations and, thus, to provide feedback to the deposition process.

In our experiment, we used a stable deposition process that produces high-density films. Refractive indices of Ta_2O_5 and SiO_2 thin-film materials have been found with high accuracy and verified using reliable results of the previous studies [23,24]. This allows us to neglect possible small offsets in layer refractive indices and to attribute the observed deviations to errors in layer thicknesses.

For indirect monitoring systems, a thickness error can be connected with variations of tooling factors and with the instability of the optical monitor. To separate these two factors we deposited standard quarter-wave high-reflectance (QWHR) coatings with the central wavelength of 800 nm and with the same layer materials and parameters of the deposition process. This test coating was chosen because, for the QWHR coatings, every monitoring chip uses the same monitoring wavelength and terminates layer depositions at the same final swing values. Thus, it is easier to check the stability of the optical monitoring system by comparing monitoring signals of every monitor chip.

The transmittance of the deposited QWHR coating is shown in Fig. 6. One can see that the discrepancy between measured and theoretical transmittance curves is obvious. When we analyzed the monitoring signals for all layer pairs, it was found that the signal extrema for the H and L layers were almost the same for each monitoring chip. The relative difference of the values was within 1% range, which could be attributed to errors in the layer thickness of not more than 0.5%. This is a rather small value, which indicates that the optical monitor in our deposition process is quite stable. Thus, we can suppose that errors in layer thickness are mainly due to the inaccuracy of the specification of tooling factors.

We performed reverse engineering of the produced QWHR coating with OptiRE software [17]. Figure 7(a) shows the fitting of measured transmittance by the theoretical transmittance when the model with random errors in thicknesses of low index layers was applied. Relative errors in all low-index layers are shown in Fig. 7(b). It is seen that the errors in all low-index layers varied gradually during the deposition procedure and that the maximum errors

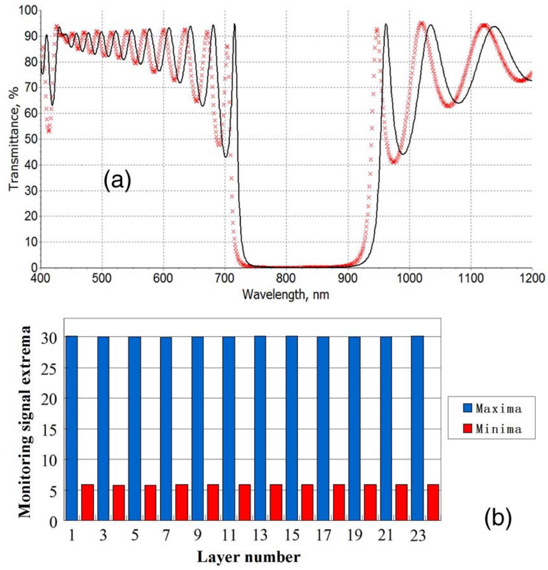

Fig. 6. (a) Comparison of the measured transmittance data (red crosses) and theoretical transmittance (solid black curve) of the standard quarter-wave coating. (b) Monitoring signal maxima (in H layers) and minima (in L layers).

are in the range of 7% of the planned theoretical layer thicknesses. The achieved excellent fitting of measurement data confirms that deviations observed in Fig. 6(a) could be attributed to the instability of tooling factors of low-index layers.

Possible instability of tooling factors was probably first indicated in [9], considering our deposition conditions we believe that the variation of the tooling

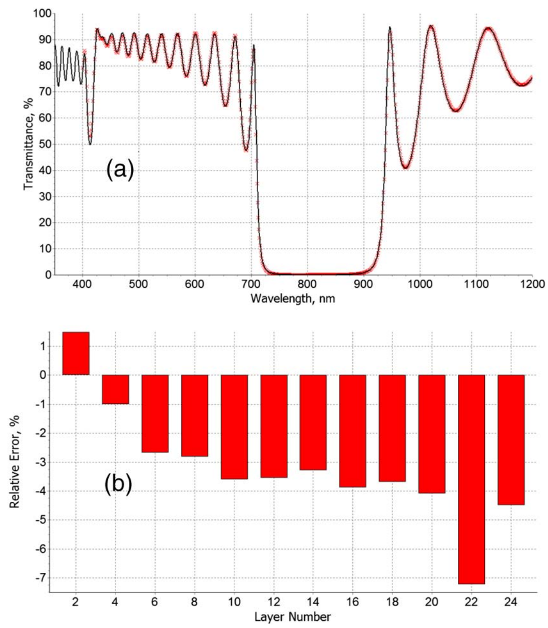

Fig. 7. (a) Fitting of measured HR transmittance (red crosses) by the model transmittance (solid curve) when the model with random errors in thicknesses of low-index layers was applied. (b) Relative random errors in low-index layers determined by the reverse engineering procedure.

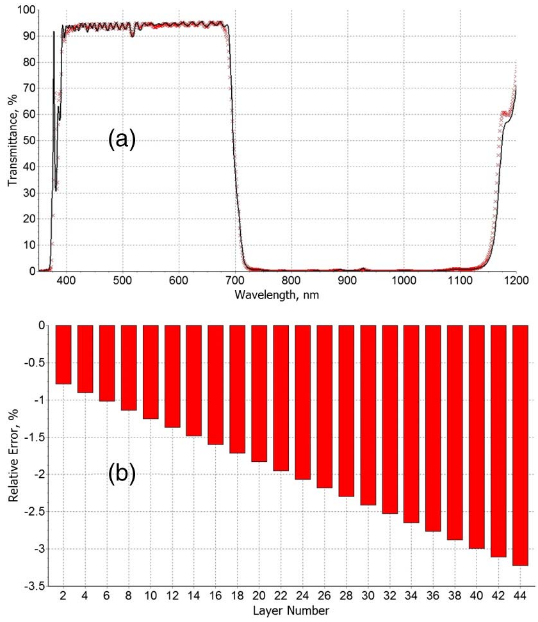

Fig. 8. (a) Fitting of measured hot mirror transmittance (red crosses) by the model transmittance (solid curve) considering linear errors in thicknesses of low-index layers. (b) Relative errors in low-index layers determined by the reverse engineering procedure.

factors of low-index layers is mainly due to the instabilities of the evaporation source and deposition rate of these layers. Based on the pattern of random errors presented in Fig 7(b), it is reasonable to assume that tooling factors of L-layers vary gradually during the deposition process. Reverse engineering of QWHR using the model of linearly varying tooling factors also provides an excellent fit of measurement data practically nondistinguishable from that presented in Fig. 7(a).

Taking into account the above results for QWHR, we performed reverse engineering of the hot mirror sample produced in the first test run using the above assumption of linearly varying tooling factors of low-index layers. Figure 8(a) shows the fitting of measured hot mirror transmittance when this model is applied. Relative errors in all low-index layers are shown in Fig. 8(b). The achieved good fitting of measurement data confirms that deviations observed in Fig. 5 could be indeed attributed to linear variation of the tooling factor in low-index layers. It is seen that the thickness errors in all low-index layers increase gradually during the deposition procedure, from 0.7% to the maximum errors of about 3.5% of planned theoretical layer thicknesses.

5. Redeposition with Modified Tooling Factors

In order to verify the reliability of our error analysis and reverse engineering results, we produced new sample of the hot mirror without changing monitoring parameters of high-index layers but with tooling factors of low-index layers linearly varying from 0.92 to 0.95. In Fig. 9, we compare the measured transmittance data of the sample produced using this monitoring approach and theoretical transmittance data. In this figure, an excellent agreement between theoretical and experimental data is observed, especially in the cutting edge and the reflection band. The obtained result confirms that the linear variation of tooling factors of low-index layers was the main inaccuracy factor in the first deposition run.

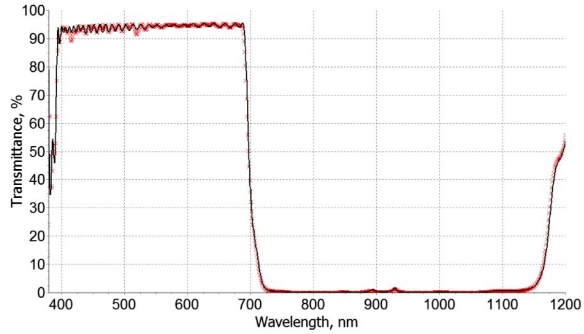

Fig. 9. Comparison of the measurement transmittance data (red crosses) and the theoretical transmittance (solid black curve) of the hot mirror in the second coating run.

6. Conclusion

In summary, we presented the advantages and challenges of the optical coating production with the indirect monochromatic monitoring. We demonstrated that the indirect monitoring using separate monitoring chips for each pair of H/L layers entirely eliminates the cumulative effect of thickness errors. It was shown that the main challenge of indirect monitoring is an accurate determination of the tooling factors for the deposited materials. The preliminary depositions of single layers and the reverse engineering of deposited multilayer samples helped us to accurately calibrate tooling factors of the monitoring procedure. Based on the feedback provided by the reverse engineering procedure, we performed the deposition experiment with a linearly varying tooling factor of low-index material and obtained excellent correspondence with the theoretical spectral performance. This research can be applied to similar deposition systems equipped with an indirect monochromatic monitoring device.

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