Adaptive manufacturing of high-precision optics based on virtual deposition and hybrid process control techniques

H. Ehlers*, **S. Schlichting, C. Schmitz, and D. Ristau**

Laser Zentrum Hannover, Hollerithallee 8, 30419 Hannover, Germany

**E-mail: h.ehlers@lzh.de*

Received October 30, 2009

The challenge in rapid production of high-precision optical coatings is the need to realize a variety of complex coating designs in one process environment. Two approaches to enhance a stable deposition process are presented. First, a virtual deposition system is applied for a pre-selection of coating designs that result in increased process stability using optical broadband monitoring strategies. Second, optical broadband monitoring is combined with additional quartz crystal sensors to realize a hybrid process control for improving layer thickness accuracy. Finally, a successful combination of both approaches is demonstrated by comparative studies on virtual and real deposition processes.

OCIS codes: 310.0310, 310.1860.

doi: 10.3788/COL201008S1.0062.

Under routine production conditions, iterative optimization cycles are often needed if varying applications demand very different highly complex coating designs. This applies particularly if the process control requires a control strategy development on an individual basis. In contrast, the adaptive manufacturing concept should enable a linear production chain without additional consumption of resources by test runs. On one hand, precision and yield can be increased by choosing multilayer designs with a higher chance of success. This decision making can be supported by sophisticated simulation software. Therefore, an effective virtual deposition system will be presented. On the other hand, an enhanced process control system for layer thickness determination is essential to reduce the waste. This second approach involves a hybrid combination of optical and non-optical process control without the need for individual (design-dependent) control strategies. In the present contribution, an optical broadband monitoring (BBM) system, which evaluates *in situ* taken transmittance spectra, is the key component in both approaches. The BBM system allows for a fully automated process control based on absolute transmittance values measured directly on the moving substrates, as well as an online computation of these data for a precise thickness determination.

This letter is organized as follows. Firstly, the concepts of the virtual deposition system and the hybrid process control will be outlined. The hybrid concept is partly based on the alternating use of BBM and quartz crystal monitoring for different layers in the stack, but mainly on a new algorithm merging the two measurements to stabilize the optical monitoring. Subsequently, the results of real and virtual deposition processes will be compared to prove the significance of the simulation results. Finally, an experimental example will document the positive effect of the combination of BBM and quartz crystal monitoring.

The core idea of the virtual deposition system is the use of the original process control software in combination with a simulation of layer growth and optical measurement[1,2]. In the first step, the deposition simulation is based on the given optical constants and rates for the employed layer materials. For each simulated measurement cycle, a transmittance spectrum corresponding to the actual layer thickness is calculated and used as input for the BBM software. In the second step, the deviations caused by the main sources of error have to be considered. Therefore, the optical constants (index of refraction, extinction coefficient), as well as the deposition rates, are varied by defined error parameter sets. Furthermore, the simulation of the measured spectral data reproduces the characteristics of the original spectrometer setup (noise, wavelength resolution). Besides random errors, the error parameter sets include systematic effects, such as offsets or drifts.

Figure 1 shows the graphical user interface of the virtual deposition system. It is divided into the BBM interface (left window) and the simulation control window. On one hand, the BBM displays information including transmittance spectra, target thickness, actual thickness and rate, or status messages. On the other hand, comprehensive adaptations of the process control parameters are possible, if required. A more detailed description of industrial environments in the well-proven BBM system can be found in Ref. [3]. In addition, the simulation control window allows for access to all parameters of the virtual deposition system. At present,

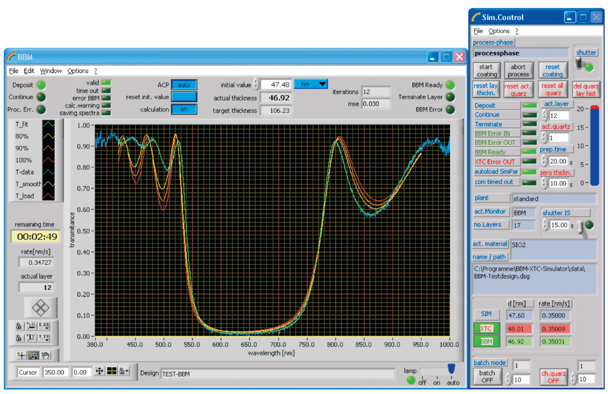

Fig. 1. Graphical user interface of the virtual deposition system (left: BBM, right: simulation control).

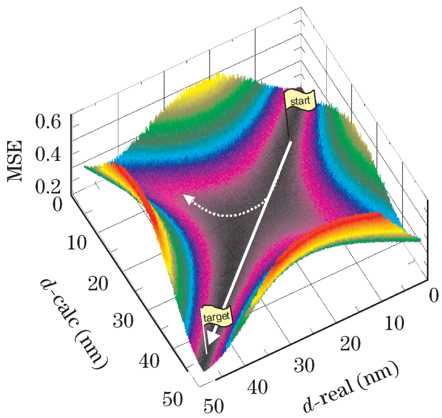

Fig. 2. Mean square error (MSE) as a function of the given layer thickness of the actual layer (d_real) and the optimization parameter (d_calc) of the BBM algorithm. Example: VIS broadband anti-reflection coating, TiO_2/SiO_2, layer 4 (calculation includes already small deviations in layers 1−3). The target point represents the target thickness of layer 4 (45.4 nm).

this virtual deposition system serves not only the BBM system but includes a complete simulation of a quartz crystal monitor as well. Depending on the chosen strategy, each individual layer can be terminated by optical or quartz crystal monitoring.

A basic way to realize hybrid process control is the alternating use of BBM and quartz crystal monitoring for different layers in the stack. In contrast, the hybrid process control in this study evaluates simultaneously the data of both monitoring systems to determine the termination point of every layer in a stack. Below, the primary concept of the hybrid system is outlined by an example of the fourth layer of a multilayer broadband anti-reflection coating for visual identification system (VIS) spectral range.

Figure 2 visualizes the basic conditions for the BBM algorithm to approximate numerically the given (actual) layer thickness, d_real, by a variation of the optimization parameter, d_calc. Plotted is the mean square error (MSE) of the corresponding two transmittance spectra (d_real: measured spectrum, d_calc: calculated spectrum from target design). Looking at the surface, an "MSE valley" from start to target point is observable, which represents the ideal path for the BBM algorithm (white arrow). Because of the minor thickness errors that occurred in the underlying layers 1−3, the MSE valley is additionally broadened in its middle. The depicted situation results in a possibility for the algorithm to leave the ideal path (dotted arrow). It should be noted that every existing path demands an increasing d_real, while an increasing or a decreasing d_calc is possible. A decreasing d_calc results in negative deposition rates, which are processed by special error handling routines.

To overcome the described possibility of error, additional information based on the quartz crystal setup for e-beam control is evaluated. In this enhanced BBM system, the algorithm is guided by quartz crystal data in a broader channel to pass critical positions successfully. Independent of this interaction, the layer can be terminated with high precision by the optical monitoring system at the final stage. This characteristic distinguishes the presented hybrid approach from related concepts in which the process is still controlled by quartz crystal monitoring[4]. Furthermore, extended error detection algorithms on the basis of the available quartz crystal data are integrated into the system. Another benefit of merging the optical and non-optical monitoring data is the possibility of refining the quartz crystal tooling at longer deposition periods.

In general, the quartz crystal data can be substituted by adapted time values within highly stable process environments. In addition to examples such as ion-beam sputtering processes with inherent superior stability[5], this requirement can be accomplished if a sufficient rate control by quartz crystal monitoring is assured. Finally, the enhanced BBM algorithm can be applied in real and simulated environments because quartz crystal simulation is implemented in the virtual deposition plant as well.

The experimental results are presented for two deposition methods: an ion-assisted deposition (IAD) process, and an ion-beam sputtering (IBS) process. The IAD process is implemented on a Leybold SYRUSpro 1100 plant equipped with a Leybold APSpro plasma source and a cryo pump. The self-constructed IBS plant is provided with a gridded high frequency (HF) ion source and two turbo pumps.

The advantages of the described concept are demonstrated by an example on the basis of two different multilayer designs. Both TiO_2/SiO_2 designs A and B fulfill identical transmittance specifications in the spectral range of 550 to 800 nm (see Fig. 3). Furthermore, it is important to notice that both designs are comparable in their characteristics in principle: 31 layers, total layer thickness ~ 2.6 μm, total thickness of $TiO_2 \sim 1.1$ μm, total thickness of $SiO_2 \sim 1.5$ μm, and no single layer thickness < 30 nm.

In a conventional approach, the design stability is tested by an analysis of the spectral deviations caused by thickness variations[6]. The results of this procedure are shown in Figs. 4(a) and (b). In multiple iterations, the individual layer thicknesses of designs A and B are varied randomly up to 1.5% (relative) and 1 nm (absolute), respectively. The blue error bars indicate the maximum spectral deviations, while the red dots represent the mean values of the deviations. Comparing the two graphs, there is no obvious difference in design stability. Looking at minor differences, the mean values suggest a slightly higher stability of design B (red dots

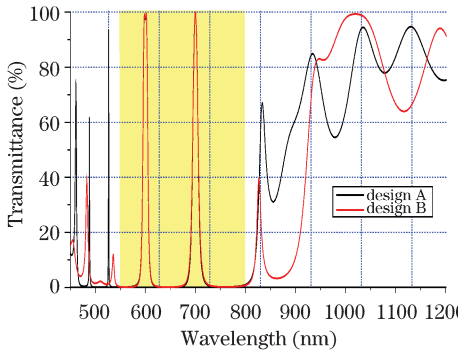

Fig. 3. Designs A and B, comparison of the transmittance spectra (no backside reflection, yellow: area covered by specifications).

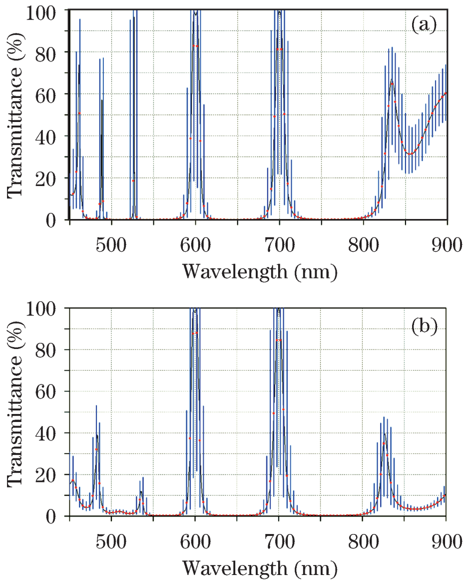

Fig. 4. Conventional design stability analysis of (a) design A and (b) design B. (blue: maximum. deviations; red: mean deviations, no backside reflection).

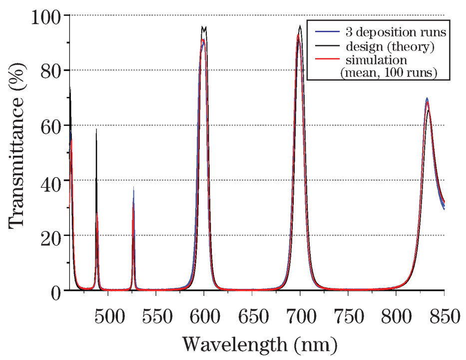

Fig. 5. Design A, IAD process, measured and simulated transmittance spectra in comparison to the target spectrum (BBM process control).

in the two transmittance peaks at 600 and 700 nm).

In contrast to the conventional design stability analysis, the described virtual deposition method produces entirely different design evaluation results. At first, the calculations are concentrated on the IAD process. Figure 5 shows the resulting transmittance spectra of three deposition runs of design A (blue), the theoretical transmittance (black), and several virtual deposition runs of design A (red). The deposition processes were not consecutively carried out with constant parameter sets without any operator interventions. Apart from the minor deviation of the experimental results from the theoretical target, no obvious discrepancy exists among the three deposition runs. Looking at the virtual deposition runs, the mean value of the 100 simulation runs is in good agreement with the measured data. Consistent with the depositions runs, the simulations exhibit high reproducibility, applying the IAD process and pertaining error parameters. The standard deviation of the simulation runs is too small to be reasonably plotted in Fig. 5 (~0.3% maximum in transmittance peaks). In this context, it should be mentioned that the present contribution is focused on systematical errors (e.g., of optical constants) as the source of layer thickness deviations. As the observed reproducible deviations considerably exceed the stochastic variations, the systematical errors are dominant under given conditions. Overall, a high stability of design A applying BBM monitoring within the IAD process can be found.

Looking at design B, the situation depicted in Fig. 6 is quite different. Again, three deposition runs, the theoretical design, and 100 averaged simulation runs are compared. In this case, a considerable discrepancy is obvious between the target spectrum and the experimental and simulation results, respectively. However, the results of the real and virtual deposition runs are again in good agreement. Consequently, design B exhibits a significantly lower design stability than design A if BBM monitoring is applied. To obtain this evaluation before the first coating run, the application of a virtual deposition system is necessary because competing design analysis methods do not reveal this result. As demonstrated above, the conventional design stability test produces the opposite result: a preference of design A contrary to reality. In principle, the accuracy of the BBM algorithm depends on the average difference of the transmittance measurements from one monitored thickness step to the next one[7]. However, in this case, design-dependent accumulation effects are dominant; therefore, the simulation is essential to evaluate design stability.

Below, the cause of the lackness of performance of design B within the IAD process is briefly discussed. Within the real, as well as the simulated deposition runs, the fault event is evidently indicated by the fact that the deposition is aborted by the process control in layer 26. Based on systematic deviations of the dispersion data, error accumulation effects result in a deterministic behavior of the BBM system, as discussed above. Following the close correspondence between simulation and reality, the virtual deposition system calculates on the basis of a dispersion data set that is in better agreement with reality than the data used by the BBM control system. In terms of process development, this knowledge could be used to refine the dispersion database for optical monitoring and multilayer design. The described error accumulation effect can be analyzed in detail employing the log files of the BBM and the virtual deposition system. Figure 7 illustrates the MSE plot (see Fig. 2) related to the crucial layer 26. Due to the accumulated thickness errors of

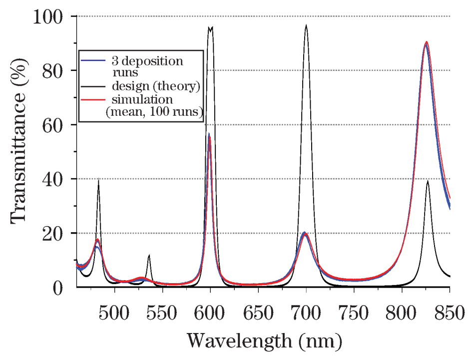

Fig. 6. Design B, IAD process, measured and simulated transmittance spectra in comparison to the target spectrum (BBM process control).

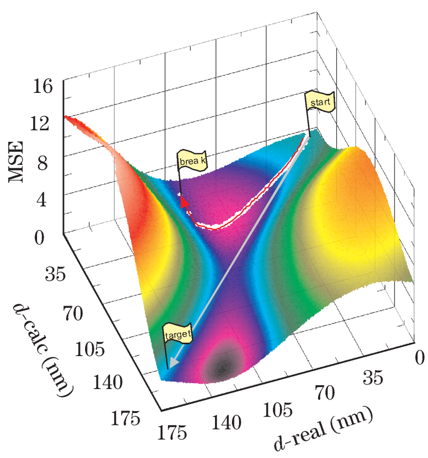

Fig. 7. Design B, explanation for the observed premature termination in layer 26. The path from the start to the breakpoint depicts the "real path" taken by the BBM algorithm. The given surface shape is a consequence of the accumulated thickness errors of layers 1 to 25.

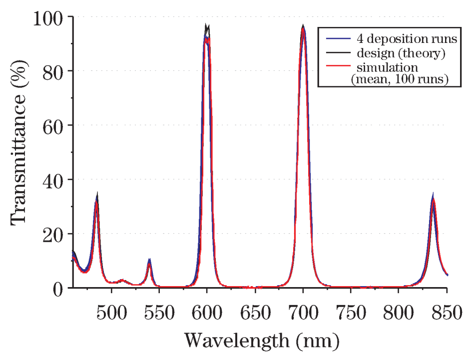

Fig. 8. Design B, IBS process, measured and simulated transmittance spectra in comparison to the target spectrum (BBM process control).

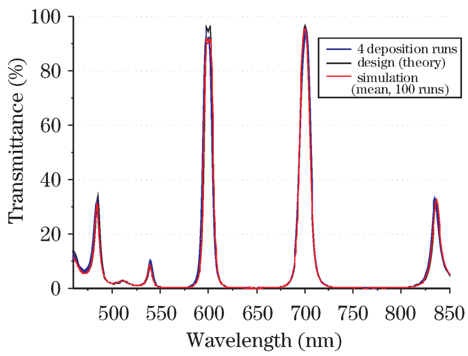

Fig. 9. Design B, IAD process, measured and simulated transmittance spectra in comparison to the target spectrum (hybrid process control).

layers 1 to 25 (and the minor dispersion aberration), the straight path from start to target point is not a distinct "deep valley." In addition, the real path taken by the BBM algorithm is plotted from the start to the termination (break) point. The observable deviation is clearly linked to the shape of the MSE surface, and finally leads to a negative rate event (hitting an "MSE hill"). However, it has to be stated that such extremely critical conditions caused by minor systematic deviations of the dispersion data are only noticed for disadvantageous designs. These designs are predetermined to be rejected by the simulation runs.

To analyze the influence of increased process stability, the design B experiment was repeated applying the IBS process. Figure 8 summarizes the IBS results of 4 depositions and 100 simulation runs. As a consequence of enhanced stability (especially of dispersion data), a significant improvement as compared to the related IAD graph (see Fig. 6) is documented in Fig. 8. Minimal differences in the IBS and IAD theoretical transmittance spectra are caused by minor design refinement due to discrepancy in dispersion data. In contrast to the IAD experiments, no premature termination was observed within the IBS process. The measured spectra, as well as the simulation results, are in good agreement with the theoretical target and exhibit a strong correlation to each other. Again, the 100 simulations and 4 deposition runs, respectively, have high reproducibility due to dominant systematic effects. Thus, as expected, plant-specific stability and variation parameters are of fundamental importance. Based on identical BBM systems, the advantage of IBS over IAD could be clearly demonstrated.

The results on the hybrid process control approach described above are related to the example of the IAD process. As depicted in Fig. 6, design B could not be successfully produced under the given IAD conditions and exclusive BBM control. Therefore, this experiment was carried out again by applying the combination of optical and quartz crystal layer thickness control. Figure 9 shows the simulation and experimental results in comparison to the theoretical design. First, it is important to note that in contrast to the previous attempt, the 31 layers could be successfully completed. Again, a good correlation between the real and the simulated deposition runs is observable. Looking at the discrepancy between the theoretical design and the experimental results, the hybrid controlled design B (Fig. 9) is comparable to the BBM exclusively controlled design A (Fig. 5). However, based on the statements above, a refinement of the dispersion data used by the optical monitoring system can be expected to increase performance in both cases.

In conclusion, an adaptive manufacturing concept comprising optical BBM was presented. On one hand, the virtual deposition system is useful as a reliable preselection tool for multilayer designs assuring a maximum yield. This significance was demonstrated by an example of two different designs fulfilling identical specifications. The pre-deposition conclusion that design A is superior to design B could only be obtained by applying the virtual deposition system. Moreover, experimental studies based on IAD and IBS processes verified the theoretical simulation results. Within the virtual deposition system, as well as in reality, the IBS, advantage of higher process stability could significantly improve the performance of critical design B. On the other hand, the hybrid process control concept combines optical and quartz crystal monitoring to an enhanced BBM system. This approach is capable of increasing the monitoring precision, especially by preventing fatal error accumulation and thus the yield significantly. Based on an example of a design which failed in the BBM monitored IAD process, the advantage of the hybrid approach could be demonstrated. Due to the fact that the virtual deposition system covers the hybrid control as well, the benefit could be proven in reality and via simulation. Consequently, the virtual deposition system assists in the choice of not only the most suitable design but also the most applicable error handling concept. Furthermore, it is a versatile tool for process development tasks such as refining dispersion data or identifying sources of deviation.

The authors thank the German Federal Ministry of Economics and Technology (BMWi) for the financial support of the research project "TACo–Tailored Automated Coating" under contract No. 16IN0407 within the framework of the InnoNet Program. Furthermore, the assistance of the VDI/VDE Innovation + Technik GmbH is gratefully acknowledged.

References

1. D. Ristau, M. Lappschies, S. Schlichting, and H. Ehlers, Proc. SPIE **7101,** 71010C (2008).
2. A. V. Tikhonravov and M. K. Trubetskov, Appl. Opt. **44,** 6877 (2005).
3. D. Ristau, H. Ehlers, T. Gross, and M. Lappschies, Appl. Opt. **45,** 1495 (2006).
4. O. Stenzel, S. Wilbrandt, D. Fasold, and N. Kaiser, J. Opt. A **10,** 085305 (2008).
5. M. Lappschies, B. Görtz, and D. Ristau, Appl. Opt. **45,** 1502 (2006).
6. H. A. Macleod, *Thin-Film Optical Filters* (3rd edn.) (Inst. of Physics Pub., Bristol, 2001).
7. M. Lappschies, P. Pfeifer, U. Schallenberg, H. Ehlers, and D. Ristau, Proc. SPIE **7101,** 71010P (2008).