Estimations of production yields for selection of a practical optimal optical coating design

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Received 21 July 2010; revised 6 October 2010; accepted 6 October 2010;
posted 7 October 2010 (Doc. ID 132086); published 24 November 2010

Modern design approaches enable one to construct a series of theoretical designs with excellent spectral properties for almost all optical coating design problems. Selection of a practical optimal design among a variety of possible theoretical designs becomes a key issue. We demonstrate how preproduction estimations of expected production yields can be used for selection of a practical optimal design. The question of reliability of such estimations is also addressed. © 2010 Optical Society of America

OCIS codes: 310.1620, 310.6805, 310.1860.

1. Introduction

For many years, starting with the publication of the famous work by Philip Baumeister [1], the concept of an optimal solution to design problems was connected with a search for the lowest possible value of a merit function estimating deviations of design spectral characteristics from target spectral characteristics. The invention of the needle optimization technique [2] and subsequent modifications of this technique [3,4] provided designers of optical coatings with effective tools for optimization of merit functions for design of all types of optical coatings. A mere optimization of a merit function is no longer a problem, but a formal search for a global minimum for merit functions has no practical sense. As an example, we can mention the detailed investigations connected with broadband antireflection coatings [5]. It is now possible to design such coatings with many tens and even hundreds of layers and to obtain lower and lower merit function values. It is, however, not practical to increase a number of design layers when a decrease of the merit function becomes too small [5].

Obviously, practical demands should be somehow incorporated in the process of designing an optical coating. It is worth noting that various practical demands were included in formulations of all design contest problems at the most recent OIC meetings [6–11]. Unfortunately, it is impossible to incorporate all practical demands in a single merit function used in a design procedure. This fact becomes obvious as soon as we recognize a key role of design total optical thickness. In one of his works, J. Dobrowolski states that "a certain minimum overall optical thickness is required for a solution to a given problem no matter what design method is employed" [12]. It turns out that design total optical thickness is an even more important parameter for achieving low merit function values than the total number of design layers [13]. As a result of this understanding, the gradual evolution version of the needle optimization technique has been developed [4]. This version provides an optical coating engineer with a set of designs having various combinations of such principal parameters as merit function value, number of design layers, and design total optical thickness. These designs have decreasing merit function values and increasing values of two other parameters. An ability to obtain a set of theoretical designs with

0003-6935/11/09C141-07$15.00/0

permanently improving spectral properties but growing complexity is the main feature of modern design approaches. Having such a set of designs at his disposal, an optical coating engineer is able to select a practical optimal design.

Another important feature of modern design approaches is an ability to look for multiple solutions with close combinations of principal design parameters [4]. It turns out that such solutions exist for many types of design problems, such as in design of hot mirrors, cold mirrors, edge filters, passband filters, etc. From a formal point of view, multiple solutions are nearly equivalent because they have close merit function values and nearly the same numbers of layers and total optical thicknesses. An existence of multiple solutions with close combinations of principal design parameters also requires concentrating attention on selection of a practical optimal design from a set of possible theoretical designs.

As mentioned above, it is impossible to formalize the concept of a practical optimal design. Selection of a specific practical optimal design is tightly connected with the deposition process being used for coating production, the monitoring technique applied for controlling layer thicknesses, cost considerations, and so on. A very useful set of information in this regard is provided by preproduction error analysis of various theoretical designs involving computational experiments aimed at simulating real production runs [14–19]. Computational manufacturing experiments are also useful for selecting of an optimum monitoring strategy for a given production environment [14,18,19].

In Ref. [14], the possibility of using computational experiments for estimating manufacturing yields was demonstrated. Performance of modern computers has increased significantly since publication of that work and it is now possible to perform multiple computational manufacturing experiments with several theoretical designs and various monitoring strategies. It is also possible to simulate all of the main factors causing production errors in real production runs [17–19]. This makes production yield estimations more relevant and allows use of these estimations in selection of the most practical design.

For computational estimation of production yields, one ought to specify some criteria that allow us to distinguish between successful and unsuccessful computational experiments. For this purpose, special targets specifying an allowed corridor of variations from target spectral characteristics can be used [20]. Experiments with spectral characteristics lying inside such corridors are considered as successful ones. A production yield can be then estimated as a ratio between the number of successful experiments and the total number of experiments [18–22].

The above approach to production yield estimations requires, however, determining how many computational experiments one should perform to obtain reliable yield estimations. It was indicated in Ref. [19] that it may be not sufficient to perform several tens of computational manufacturing runs, and many more experiments may be required. Thus, in Ref. [19], 1500 computational manufacturing runs were performed for production yield estimations. Unfortunately, there are situations when performing thousands of computational experiments with several theoretical designs is still too time-consuming, even when the best modern computers are employed. These are situations where production runs with broadband optical monitoring are simulated. In Section 2 of this paper, we use some basic results from probability theory to find a reasonable number of computational experiments required for production yield estimations.

In Section 3, we demonstrate an application of production yield estimations for choosing of a practical optimal design. Several theoretical designs with ramp spectral transmittance dependencies are compared. Computational experiments with noncorrelated thickness errors and experiments simulating production runs with broadband and monochromatic optical monitoring are considered. The coating with ramp transmittance dependence is manufactured using an appropriate monitoring strategy and a design chosen based on yield estimations. Final conclusions are provided in Section 4.

2. Confidence Intervals for Production Yield Estimations

Let us denote a total number of computational experiments used for production yield estimations as N. Suppose that some criteria for distinguishing between successful and unsuccessful experiments have been already specified, and denote a number of successful experiments as M. It is natural to estimate a production yield as a ratio

$$Y = M/N. \tag{1}$$

Naturally, if the number N is increased, then Y gives a more accurate estimation of production yield. The reliability of such statistical estimation is one of the basic questions of the probability theory and mathematical statistics [23]. In terms of mathematical statistics, N is called a sample size and M is called a number of successes in this sample size. The ratio Y is called a point estimation of the probability p of successful events. Under rather wide assumptions, Y tends to p if the sample size N tends to infinity. A practical question considered in this Section is formulated as follows. What sample size N is required to approximate p value by the yield estimation Y with sufficient accuracy?

Probability theory introduces the concept of a confidence interval for point estimation Y. The point estimation Y belongs to this interval with a given probability α. This probability is called a level of confidence. Boundaries of the confidence interval p_-, p_+ are roots of the quadratic equation

$$p^2\left(1+\frac{z_\alpha^2}{N}\right) - p\left(2\,Y+\frac{z_\alpha^2}{N}\right) + Y^2 = 0, \tag{2}$$

where z_α is found from the level of confidence α using the equation

$$2\ \mathrm{erf}(z_\alpha) = \alpha, \tag{3}$$

where erf() is a well-known Gauss error function.

The width of the confidence interval $\Delta p = p_+ - p_-$ can be considered as an accuracy of point estimation Y. This accuracy depends on the sample size N, on the point estimation Y, and on the level of confidence α.

To illustrate the above concepts, let us take the level of confidence α as equal to 0.99, or 99% as a percentage. Figure 1 presents the dependencies of the width of the confidence interval on Y for three N values equal to 10, 100, and 1000. Naturally the width of the confidence interval is decreased, and the accuracy of the point estimation Y is increased respectively when the sample size is increased. Nevertheless, even for $N = 1000$, this width may be up to 0.08, or 8%. The highest width value and respectively, the poorest accuracy, corresponds to $Y = 0.5$. It is worth noting that for point estimations close to 0 and to 1, the accuracy of estimation is improved.

It is rather surprising how many experiments are required for reliable yield estimations. For example, if we want to achieve 5% accuracy for all Y values, then at least 2700 experiments are required. To achieve 1% accuracy, the total number of experiments should be more than 67 000. But these are rigorous results of probability theory and we must take them into account if we want to obtain reliable yield estimations. In Section 3 we consider practical yield estimations and discuss the choice of a realistic number of computational manufacturing experiments.

3. Practical Examples of Production Yield Estimations

We consider, as an example, the design and manufacture of a coating with spectral transmittance that varies linearly from 0% at 400 nm to 100% at 800 nm. In what follows, this target transmittance is referred to as ramp transmittance. For manufacturing of this coating, we use BK7 substrate, silicon dioxide, and niobium pentoxide as layer materials.

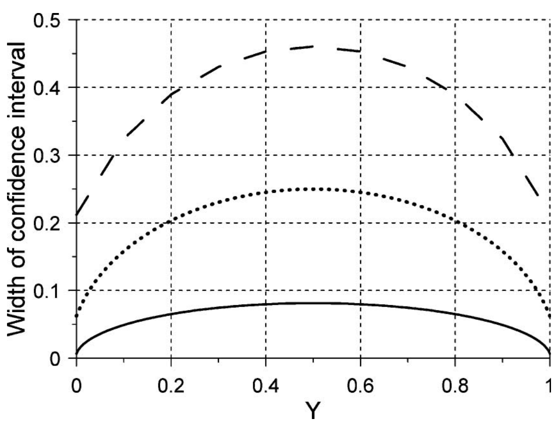

Fig. 1. Dependencies of confidence interval width on Y:$N = 1000$ (solid curve), $N = 100$ (dotted curve), and $N = 10$ (dashed curve).

The considered problem allows obtaining multiple designs with close combinations of merit function values, numbers of design layers, and design total optical thicknesses. Figure 2 shows refractive index profiles of four such designs, labeled as Ramp 18a, Ramp 18b, Ramp 19, and Ramp 21 with the numbers 18a, etc. indicating total numbers of design layers. The letters a, b are used to distinguish between two different 18 layer designs. The designs are obtained using the design approach outlined in Ref. [4]. This approach is based on generation of a special set of random starting designs and application of efficient local optimization and needle optimization routines.

All four designs have excellent spectral properties. As an example, Fig. 3 presents the transmittance of the design Ramp 21. Figure 3 also presents one of the range targets used for yield estimations discussed below.

For the production of a coating with ramp transmittance, we had two deposition plants at our disposal: a magnetron-sputtering Leybold Optics Helios machine with time monitoring of layer thicknesses, and a Leybold Optics Syrus Pro 710 plant with broadband optical monitoring. For choosing a practical optimal design and an appropriate monitoring strategy, we estimated production yields for the four designs shown in Fig. 2, using computational experiments with different types of production errors. For the case of time monitoring, statistical tests with noncorrelated random thickness errors were performed. For the case of broadband optical monitoring, computational manufacturing experiments were accomplished. Error factors simulated in these experiments are listed below. For a more complete comparison of various monitoring strategies, we also considered computational manufacturing experiments with monochromatic optical monitoring. A well-known strategy based on the choice of the most sensitive monitoring wavelength [24,25] was used in these experiments. In the following text this strategy is referred to as the MSW strategy.

In practice, a variety of different algorithms can be used to process measurement data obtained by broadband and monochromatic monitoring approaches. It is possible, however, to indicate two major types of algorithms that are most often employed with monitoring approaches of these two

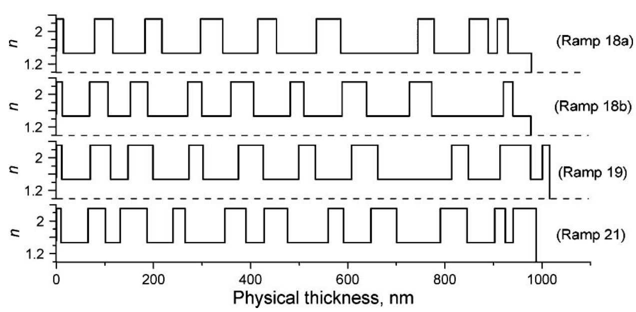

Fig. 2. Refractive index profiles of four designs with ramp transmittance in the spectral region from 400 to 800 nm; reference wavelength for refractive index values is 600 nm.

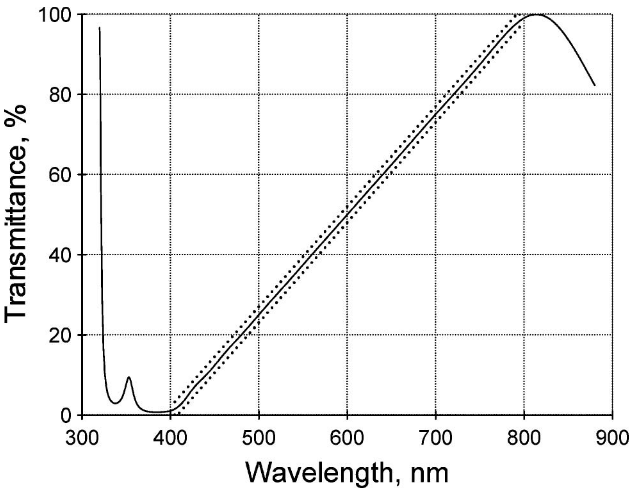

Fig. 3. Transmittance of the Ramp 21 design and the corridor of $\pm 2\%$ deviations from the target transmittance.

types. In the case of broadband optical monitoring algorithms calculating film thickness from broadband spectra are typically used nowadays [18,19]. In our experiments with broadband optical monitoring we use an algorithm of this type presented in Ref. [26]. The most widely used monochromatic monitoring strategies and, in particular, the MSW strategy are so-called level monitoring strategies [27]. In the case of level monitoring, film thickness is not calculated from monitoring data and layer deposition is terminated when the monitoring signal achieves a predicted termination level specified in a monitoring spreadsheet. In our experiments with monochromatic monitoring, we use level monitoring with the monitoring spreadsheet specified according to the MSW strategy.

For estimation of production yields, we use three range targets that specify the allowed corridors of deviation from the target ramp transmittance in the spectral region from 405 to 795 nm. These corridors are set as $\pm 1\%$, $\pm 1.5\%$, and $\pm 2\%$. Computational experiments resulting in transmittances that lie inside a specified corridor are considered as successful ones. Naturally, production yields are expected to be higher for wider corridors of allowed deviations from the ramp transmittance.

Computational manufacturing experiments simulating production runs with broadband optical monitoring are the most time-consuming experiments. For this reason, selection of a realistic number of experiments is especially important in this case. Simple practical speculations allow one to avoid unnecessary experiments. Figure 1 shows that the highest width of the confidence interval and, respectively, the poorest accuracy of production yield estimations corresponds to intermediate Y values. But if a production yield is not high enough, then it is not practical to estimate it with a high accuracy. It is obvious that one needs more accurate estimations for production yields of those designs that provide Y values close to 1. Fortunately, the theory predicts much better accuracy of estimations for such Y values than for intermediate Y values.

For each of the designs depicted in Fig. 2, experiments with broadband optical monitoring were performed for the three corridors of allowed deviations discussed above. Thus, in all, 12 series of experiments were performed. Total numbers of experiments in these series were different and were based on the above considerations of sufficient accuracy of yield estimations. The initial number of experiments in all series was 100. For experiments with yield values higher than 85%, the numbers of experiments was then increased to 1000, which provided much better accuracy of yield estimations.

In our experiments, all of the major factors causing production errors in a real deposition chamber were simulated. Instabilities in layer material deposition rates were represented by random processes with correlation times of 3 s for both materials. The mean rates for the low and high index materials were 0.5 nm/s and 0.4 nm/s, respectively. The root mean square (rms) fluctuations of these rates were specified as 0.1 nm/s and 0.05 nm/s. Inaccuracies in closing shutters were also simulated. Rms errors in terminating layer deposition were equal to 0.5 s. Broadband optical monitoring data were transmittance data acquired in the spectral region from 400 to 800 nm with a wavelength step of 1 nm. The time interval between broadband measurements was 4 s. For each scan of broadband monitoring data, random errors with a rms level of 1% were simulated.

Estimated production yields Y and respective confidence intervals $[p_-, p_+]$ are presented in Table 1. As discussed above, $[p_-, p_+]$ boundaries for Y values higher than 85% are estimated using increased

Table 1. Estimated Production Yields and Respective Confidence Intervals for Different Levels of Allowed Transmittance Deviations from the Target Ramp Transmittance: Experiments with Broadband Optical Monitoring, Numbers of Experiments are Equal to 100 if $Y < 85\%$ and to 1000 if $Y > 85\%$

	Estimated Production Yields and Respective Confidence Intervals					
	$\pm 1\%$		$\pm 1.5\%$		$\pm 2\%$	
Design	Y (%)	$[p_-, p_+]$ (%)	Y (%)	$[p_-, p_+]$ (%)	Y (%)	$[p_-, p_+]$ (%)
Ramp 18a	56	[43.2;68.0]	82	[70.2;89.8]	94.3	[92.1;95.9]
Ramp 18b	54	[41.3;66.2]	92.3	[89.8;94.2]	99.0	[97.8;99.5]
Ramp 19	40	[28.4;52.9]	83	[71.3;90.5]	91.3	[88.7;93.3]
Ramp 21	21	[12.5;33.1]	51	[38.4;63.4]	61	[48.1;72.5]

Table 2. Estimated Production Yields and Respective Confidence Intervals for Different Levels of Allowed Transmittance Deviations from the Target Ramp Transmittance: Experiments with Monochromatic Optical Monitoring Strategy MSW, Numbers of Experiments are Equal to 1000

	Estimated Production Yields and Respective Confidence Intervals					
	$\pm1\%$		$\pm1.5\%$		$\pm2\%$	
Design	Y (%)	$[p_-,p_+]$ (%)	Y (%)	$[p_-,p_+]$ (%)	Y (%)	$[p_-,p_+]$ (%)
Ramp 18a	43.3	[39.3;47.4]	77.1	[73.5;80.3]	92.9	[90.5;94.7]
Ramp 18b	78.8	[75.3;81.9]	97.8	[96.2;98.7]	100	[99.3;100]
Ramp 19	41.7	[37.7;45.8]	71.7	[67.9;75.2]	89.4	[86.6;91.7]
Ramp 21	35.5	[31.7;39.4]	70.5	[66.7;74.1]	87.9	[85.0;90.3]

numbers of computational experiments. One can see that in the case of broadband optical monitoring, the best Y values are provided by the design Ramp 18*b*.

Table 2 presents estimated production yields with confidence intervals for the case of optical coating production with monochromatic monitoring strategy MSW and transmittance measurement data. Except for the level of measurement errors, the same error factors as in the previous case were simulated. Random errors in monitoring data in the case of coating production with monochromatic optical monitoring are much more serious than they are in the case of production with broadband optical monitoring [25]. For this reason, a much lower level of random errors was specified, 0.05%, compared with the previous case. Time intervals between acquisitions of monochromatic transmittance data were 1 s. Computational manufacturing experiments with monochromatic optical monitoring are less time-consuming than analogous experiments with broadband optical monitoring. For this reason, 1000 experiments were conducted in each series of experiments. According to the results presented in Table 2, the superiority of the design Ramp 18*b* over other designs is even more evident than in the case of broadband optical monitoring.

Table 3 presents estimated production yields with confidence intervals for the case of noncorrelated random errors in layer thickness. This case is the simplest type of preproduction error analysis because errors in layer thickness are simulated directly and are not obtained in the course of a computational manufacturing experiment based on error factors inherent in the processes of production and measurement [24]. Computational experiments with random errors in layer thickness are much faster than any type of computational manufacturing experiments simulating production runs with optical monitoring; for this reason, we performed 5000 such experiments in each series of experiments. For this reason, the confidence intervals in Table 3 are narrower than in the two previous tables.

An assumption of noncorrelated random errors in layer thicknesses is relevant for the case of optical coating production with well-calibrated time monitoring when systematic errors in layer thicknesses caused by inaccurate calibrations of deposition rates have already been eliminated. Even with an accurate calibration of a deposition rate, there may be some additional thickness errors caused by calibration drift of a quartz crystal in time. We did not simulate errors of this type, however, because in the case of our magnetron-sputtering process, we never observed noticeable calibration drifts. In principle, such drifts can be caused by contamination effect and target oxidations, and with other deposition processes, it may be reasonable to simulate them in computational manufacturing experiments.

In the computational experiments used for the estimations in Table 3, we assumed that the remaining random errors were distributed by normal laws with standard deviations equal to 0.5% of theoretical layer thicknesses. Table 3 shows that now we have two designs, namely, the designs Ramp 18*b* and Ramp 21, that clearly demonstrate their superiority over other designs. Ramp 21 is a bit more attractive because it has somewhat better production yield with a $\pm1\%$ corridor of allowed transmittance deviations from the ramp transmittance.

Here it is necessary to make one comment concerning the results presented in Tables 1–3. It is evident that computational manufacturing is not able to simulate the coating production completely. Thus the confidence interval margins should not be considered

Table 3. Estimated Production Yields and Respective Confidence Intervals for Different Levels of Allowed Transmittance Deviations from the Target Ramp Transmittance: Experiments with Noncorrelated Random Errors in Layer Thicknesses, Numbers of Experiments are Equal to 5000

	Estimated Production Yields and Respective Confidence Intervals					
	$\pm1\%$		$\pm1.5\%$		$\pm2\%$	
Design	Y (%)	$[p_-,p_+]$ (%)	Y (%)	$[p_-,p_+]$ (%)	Y (%)	$[p_-,p_+]$ (%)
Ramp 18a	44.7	[42.9;46.5]	85.1	[83.8;86.4]	97.5	[96.9;98.0]
Ramp 18b	51.9	[50.1;53.7]	92.0	[91.0;92.9]	99.1	[98.7;99.4]
Ramp 19	47.1	[45.3;48.9]	86.7	[85.4;87.9]	98.0	[97.4;98.5]
Ramp 21	55.7	[53.9;57.5]	92.5	[91.5;93.4]	99.0	[98.6;99.3]

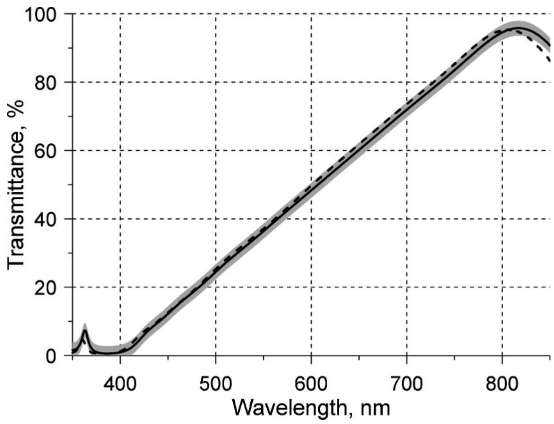

Fig. 4. Measured transmittance of the 21 layer coating (dashed curve), theoretical transmittance of the Ramp 21 design (solid curve), and the corridor of ±2% deviations from the theoretical transmittance (gray area).

as absolutely accurate values. Nevertheless, these margins allow one to compare confidence levels of yield estimations for different designs. At the same time, computer simulations of real production runs become more and more accurate due to a better understanding of error factors and their representation in computational manufacturing runs [18,19]. With the growing accuracy of simulation software, the significance and accuracy of computational yield estimations will also grow.

Because of a better practical experience with the magnetron-sputtering process, we selected the Helios machine for the production of ramp coating based on the Ramp 21 design. The machine is equipped with two TwinMags magnetrons and a plasma source for plasma ion-assisted reactive middle-frequency dual-magnetron sputtering. The system was pumped by turbo-molecular pumps to 10^{-6} mbar pressure before the deposition. Argon and oxygen were supplied for both magnetrons. In the magnetron cathodes, Nb and Si targets were used. The electric power of the Si cathode was 4500 W and the power of the Nb cathode was 3500 W. The power applied to the Nb cathode was not constant because it operated in the oxygen control mode, which guaranteed stable film properties. The gas pressure was 10^{-3} mbar during the sputtering process. Oxygen was fed near the targets to oxidize sputtered films. The distance from the targets to the substrates was 100 mm. The purity of the Si target was 99.999% and that of the Nb target was 99.9%. By changing the electric power applied to the cathode, it was possible to increase or decrease the sputtering rate. We found that quality of films of both materials was degrading at high rates. Good quality was achieved at the rates of around 0.5 nm/s for both materials.

In Fig. 4, the measured transmittance of the deposited coating is compared with the theoretical transmittance of the Ramp 21 design. One can observe a good correspondence between the measured and theoretical data. The measured transmittance spectrum fits into a ±2% corridor of deviations from the theoretical transmittance spectrum. Theoretical transmittance in Fig. 3 differs slightly from that in Fig. 4 because reflectance from the substrate back side is taken into account in the case of Fig. 4.

4. Conclusions

The outstanding efficiency of modern design techniques allows one to obtain a series of excellent theoretical designs for any optical coating design problem. The choice of a practical optimal design from a variety of possible theoretical designs becomes a key issue in raising efficiency of optical coating production. Preproduction estimations of expected production yields of different designs may play an important role in selection of a practical optimal design and decreasing the number of test production runs in a real production situation. Computational manufacturing, or computer simulation of deposition and monitoring processes, is the most relevant tool for the preproduction yield estimations and selection of the most manufacturable design. To achieve reliable yield estimations, hundreds and even thousands of computational experiments may be required, but performing these large numbers of experiments is possible even when production runs with broadband optical monitoring are simulated.

There is a strong need for further studies in the field of computer simulation of deposition and monitoring processes. Deeper understanding of error factors inherent in these processes will allow simulation of real production runs with high accuracy. The main goal of further studies is reduction of production costs and the time frame for developing new products, by eliminating test production runs and replacing them with computational manufacturing experiments.

This work was supported by the Russian Foundation for Basic Research (RFBR), projects 09-02-13607, 10-07-00480a (http:\\www.rfbr.ru) and the Deutsche Forschungsgemeinschaft (German Research Foundation) (DFG) Cluster of Excellence, Munich-Centre for Advanced Photonics (http:\\www.munich-photonics.de).

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