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CORRELATION OF ERRORS IN OPTICAL COATING PRODUCTION WITH BROAD BAND MONITORING

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We propose a robust estimate that can be used for the prediction of the expected strength of thickness errors correlation in the case of optical coating production with the direct broad band monitoring of a deposition process. A practical application of this estimate requires statistical analysis. We introduce a computationally efficient simulator of thickness errors that have a random character and are able to adequately represent the correlation of thickness errors by a monitoring procedure. It is shown that the expected strength of thickness errors correlation is estimated by the random value whose distribution is close to the log-normal distribution and that the two main parameters of the log-normal probability density function can be used as the parameters characterizing the investigated effect.

Keywords: inverse problems, optical coating technology, optical monitoring, computer simulation.

1. Introduction. The importance of optical coatings for the progress in many technological areas and the main inverse problems connected with the optical coating manufacturing are discussed in detail in [1]. At the current state of the art in optical coating production, a key role is played by inverse reconstruction problems connected with monitoring the coating production. Among all the variety of monitoring techniques, the broad band monitoring (BBM) technique is considered as the most promising one [2]. This technique uses arrays of on-line measurement data obtained every several seconds and requires to solve the following two types of inverse problems: multi-parameter inverse characterization problems and one-parameter inverse monitoring problems [3]. In the first case, all or some of the accumulated measurement data are used to determine the thicknesses of already deposited layers. In the second case, the determined thicknesses of previously deposited coating layers are used by the on-line monitoring algorithms to determine a growing thickness of the currently deposited layer and to predict a layer deposition termination instant. Much attention is now being paid to improving the accuracy of both types of algorithms [4–6], but errors in thicknesses of coating layers are nevertheless inevitable.

In the case of direct monitoring, on-line measurement data are affected by the errors in thicknesses of already deposited layers. Because solutions of both types of inverse problems are based on these data, this causes a correlation of errors in thicknesses of layers of deposited coatings. This correlation has a negative consequence known as the cumulative effect of thickness errors [7]. But along with the negative effect, there is also a positive consequence of the thickness errors correlation. This is the effect of self-compensation of thickness errors [1]. It was practically shown that, due to this effect, the optical coating production can be successful even in the case of very high production errors [8]. This makes the study of thickness errors correlation extremely important for the modern optical coating technology.

A mathematical study of the effects of thickness errors correlation and self-compensation is performed in [1]. The main aims are to reveal the origin of these effects and to find how it is possible to predict their presence

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for a given optical coating design and specific parameters of the direct BBM procedure. It is shown [1] that the correlation of thickness errors related to the solution of inverse characterization and monitoring problems can be described in terms of eigenvectors of a special rectangular matrix constructed based on the discrepancy functionals of these on-line inverse problems. It is also shown that the prediction of the existence of a strong error self-compensation effect can be made by comparing the singular values of this matrix with the singular values of another rectangular matrix that additionally takes into account the solution of the inverse problem of optical coating design.

The purpose of this study is to further develop the results of [1] and to introduce a robust estimate that can be used in practice for the pre-production study of thickness errors correlation. In Section 2 we provide a brief overview of the inverse problems related to the investigated effect and propose the expression for the above-mentioned estimate. In Section 3 we consider the thickness errors simulator required for the reliable statistical study of thickness errors correlation. In Section 4, a practical application of the proposed estimate is discussed. Our final conclusions are given in Section 5.

2. The inverse problem of thickness monitoring and correlation of thickness errors. For definiteness, we consider the case of direct BBM in the transmission mode. This means that the on-line measurement data supplied by the monitoring equipment are spectral transmittance data. Let $d_1, \ldots, d_m$ be physical thicknesses of coating layers with m being the total number of coating layers. Spectral transmittance of an optical coating T depends on these parameters and is calculated using the formulas given in [1]. A more detailed consideration of the direct problem in thin film optics can be found in the book [9]. The free access to the necessary pages of this book is also available on the Internet (see [10]).

Let us start with the inverse problem of thickness monitoring. Suppose that $j-1$ layers have been already deposited and the thickness of jth layer is monitored. In the case of direct BBM, the following functional is used to predict the instant of terminating the layer deposition:

$$\Phi_j = \sum_{\lambda} \left[T_j^{\text{meas}}(d_j, \lambda) - T_j^{\text{theor}}(\lambda)\right]^2. \tag{1}$$

Here λ is the wavelength of the incident light, T_j^{meas} is the measured transmittance spectrum provided by optical monitoring equipment, and T_j^{theor} is the theoretical transmittance spectrum at the end of the jth layer deposition calculated using the theoretically planned layer thicknesses. In Eq. (1) the summation is performed over the measurement wavelength grid.

By $d_1^t, \ldots, d_m^t$ we denote the theoretically planned layer thicknesses. Their values are obtained by solving the inverse synthesis problem [11]. The measured transmittance T_j^{meas} varies with an increase in the thickness d_j. Below we indicate the dependence of T_j^{meas} on d_j, but omit the indication of its obvious dependence on the wavelength λ. The measured transmittance can be written as

$$T_j^{\text{meas}}(d_j) = T_j\big(d_1^a, \ldots, d_{j-1}^a, d_j\big) + \delta T_{\text{meas}},$$

where $d_1^a, \ldots, d_{j-1}^a$ are the actual thicknesses of the previously deposited layers and δT_{meas} are the errors in measured transmittance data.

The measured spectra are recorded on-line with small time intervals between measurements so that only small layer fractions are deposited between measurement instants. In general, the deposition of the jth layer is terminated when the functional expressed by (1) achieves its minimum value. There are various tricks [3, 4, 12, 13] to increase the stability of layer thickness monitoring by taking into account additional information during minimizing this functional, but they are not essential for our considerations and we assume that the thickness d_j of the jth layer corresponds to the minimum of the functional

$$\Phi_j(d_j) = \min_d \sum_{\lambda} \Big[T_j\big(d_1^a, \ldots, d_{j-1}^a, d\big) + \delta T_{\text{meas}} - T_j\big(d_1^t, \ldots, d_m^t\big)\Big]^2. \tag{2}$$

Naturally, the thickness d_j of the jth deposited layer differs from the theoretically planned value d_j^t: $d_j = d_j^t + \delta d_j$. Here δd_j is the error in the jth layer thickness.

Let δd_i be the errors in the thicknesses of the previously deposited layers: $\delta d_i = d_i^a - d_i^t$, $i = 1, \ldots, j-1$. The monitoring of the coating production based on condition (2) causes the correlation of thickness errors at each step of the deposition procedure.

In [1] it is shown that the correlation of thickness errors at the jth step of the deposition process can be represented by the condition of reaching a minimum by the quadratic form:

$$\big(D^j\big)^T C^j D^j \to \min. \tag{3}$$

Here $D^j = \{\delta d_1, \ldots, \delta d_{j-1}, \delta d_j\}^T$ is the column vector of thickness errors at the jth deposition step and C^j is the matrix

$$C^j = \left\| \sum_{\lambda} \frac{\partial T^j}{\partial d_i} \frac{\partial T^j}{\partial d_k} \right\| .$$

Here $\partial T^j / \partial d_i$ are the transmittance derivatives of the subsystem consisting of j layers. These derivatives are calculated at the theoretical layer thicknesses d_i^t, $i = 1, \ldots, j$.

When the deposition process is over, the errors in all the layer thicknesses turn out to be correlated. To describe the correlation process as a whole, the following transformations are made in [1] with all conditions (3).

First, the conditions expressed by (3) are transformed to the form

$$\left(D^j\right)^T P^j \, V^j \left(P^j\right)^T D^j \to \min . \tag{4}$$

Here V^j are the diagonal matrices whose elements are the eigenvalues λ_j^i of the matrix C^j in descending order and P^j are the matrices whose columns are the eigenvectors of the matrix C^j.

The conditions expressed by (4) can also be written as

$$\sum_{i=1}^{j} \lambda_i^j \left[\left(P_i^j\right)^T D^j \right]^2 \to \min . \tag{5}$$

Here P_j^i are the columns of the matrix P^j (i.e., the eigenvectors of the matrix C^j). Let $p_1^{ij}, \ldots, p_j^{ij}$ be the components of this vector. Introducing the row vector W_{ij}

$$W_{ij} = \sqrt{\lambda_i^j} \, \left\{ p_1^{ij}, \ldots, p_j^{ij}, 0, \ldots, 0 \right\}$$

and the error vector

$$\Delta = \{\delta d_1, \ldots, \delta d_m\}^T,$$

we can rewrite conditions (5) as

$$\sum_{i=1}^{j} (W_{ij} \Delta)^2 \to \min . \tag{6}$$

There are $m - 1$ conditions (6), since the correlation of thickness errors starts at the deposition of the second coating layer. One of the main results of [1] is the introduction of the matrix W whose rows are the vectors W_{ij} for all $j = 2, \ldots, m$ and all $i = 1, \ldots, j$. This is a rectangular matrix with the dimensions $k \times m$, where $k = (m-1)(m+2)/2$. According to [1], the correlation of thickness errors leads to a decrease of the norm of the vector $W\Delta$. The further results of [1] are based on the singular value decomposition (SVD) of the matrix W and the final conclusions of [1] are made in terms of singular values of rectangular matrices.

The aim of our considerations is to further develop the results of [1] by introducing a robust estimate that can be used in practice for the pre-production study of thickness errors correlation. To achieve this aim, we also use the SVD of the matrix W:

$$W = U \Sigma V^T . \tag{7}$$

Here U and V are the orthogonal matrices whose dimensions are $k \times k$ and $m \times m$, respectively; Σ is a rectangular matrix whose dimensions are $k \times m$ and whose nonzero elements are situated on its diagonal. These elements are called the singular values of the matrix W. We denote them by $\sigma_1, \ldots, \sigma_m$.

Using the SVD expressed by (7), we can write

$$\|W\Delta\|^2 = \sum_{i=1}^{m} \sigma_i^2 \left(V_i^T \Delta\right)^2, \tag{8}$$

where V_i are the column vectors of the orthogonal matrix V.

Now is the time to make some comments about the error vector Δ. Errors in thicknesses of optical coatings are caused by multiple random factors connected with the coating deposition process and by the thickness monitoring procedure. These factors include the instabilities of deposition rates of thin film materials, the fluctuations of thin film refractive indices inside the deposition chamber, the random errors in measurement data, and much more [14]. For this reason, despite the correlation of errors, the error vector Δ has nevertheless a random character and can vary from one deposition process to another. This means that our further considerations require statistical analysis. The following statement is useful for such analysis.

Statement. Consider the square norm $\|W\Delta\|^2$ on a sphere of unit radius $\|\Delta\| = 1$. The mean value of this square norm is given by the equation

$$\langle \|W\Delta\|^2 \rangle = \frac{1}{m} \sum_{i=1}^{m} \sigma_i^2. \tag{9}$$

Let Δ^0 be an error vector obtained in the course of coating deposition with direct BBM. In accordance with [1], the square norm $\|W\Delta^0\|^2$ must be small in the case of thickness errors correlation. Equation (8) gives that

$$\|W\Delta^0\|^2 = \sum_{i=1}^{m} \sigma_i^2 \left(V_i^T \Delta^0\right)^2.$$

To estimate the smallness of the square norm $\|W\Delta^0\|^2$, it is natural to compare it with the mean value of the square norm $\|W\Delta\|^2$ on a sphere of unit radius (see Eq. (9)). For such comparison, of course, the error vector Δ^0 must be normalized to the unit vector. On the basis of these considerations, we introduce the following expression for estimating the strength of thickness errors correlation:

$$\alpha = \|W\Delta^0\|^2 \Big/ \left[\frac{1}{m} \sum_{i=1}^{m} \sigma_i^2\right]. \tag{10}$$

It is natural to suppose that, in the case of a strong correlation of thickness errors, the value of α is essentially smaller than 1. We can also say that the correlation is stronger when α is smaller. The practical application of the introduced estimate will be considered in Section 4.

3. Thickness errors simulator. It was already indicated that the errors in coating layer thicknesses have a random character and that, for this reason, the analysis of thickness errors correlation requires statistical analysis. It was also mentioned that the thickness errors are caused by various factors connected both with the coating deposition process and with the thickness monitoring procedure. In recent years, a special attention was paid to the study of thickness errors using computer simulations of optical coating production [13–15]. The corresponding computational experiments got the name of computational manufacturing of optical coatings. In principle, these experiments can be used to generate various sets of thickness errors. Computational manufacturing experiments are much faster than real production runs and, using modern simulation tools [10], one can perform dozens of such experiments. However, such a number of experiments is completely inadequate for the statistical analysis based on estimate (10). This will be clearly demonstrated in Section 4.

This section of the paper is devoted to the description of a simplified simulation tool that can be used to generate hundreds of thousands and even millions of thickness error vectors in a realistic time. The aim is to generate error vectors that have a random character and are able to adequately represent the correlation of thickness errors by direct BBM. The possibility of using the introduced tool instead of much more precise computational manufacturing experiments will be justified in Section 4.

Recall that the direct BBM procedure is based on the minimization of functional (2):

$$\Phi_j(d_j) = \min_d \sum_\lambda \Big[T_j\big(d_1^a, \ldots, d_{j-1}^a, d\big) + \delta T_{\text{meas}} - T_j\big(d_1^t, \ldots, d_m^t\big)\Big]^2.$$

Monitoring of the coating production based on this criterion causes the correlation of thickness errors at each step of the deposition procedure. If we ignore the presence of random measurement errors, then the minimum of the above functional is achieved for

$$\delta d_j = -\sum_{\{\lambda\}} \left(\sum_{i=1}^{j-1} \frac{\partial T_j}{\partial d_i} \frac{\partial T_j}{\partial d_j}\, \delta d_i\right) \Big/ \sum_{\{\lambda\}} \left(\frac{\partial T_j}{\partial d_j}\right)^2. \tag{11}$$

This equation describes the correlation of thickness errors in a simplified form.

There are multiple random factors causing thickness errors, but in the simplified simulator we present all of them in the form of a random component of each thickness error δd_j. On the whole, the algorithm for simulating the thickness errors is formulated as follows.

1. Let $j = 1$. In the first deposited layer, the thickness error is set as $\delta d_1 = \nu_1$, where ν_1 is a normally distributed random error.
2. Redefine $j = j + 1$.
3. Define δd_j according to Eq. (11).
4. Redefine $\delta d_j = \delta d_j + \nu_j$, where ν_j is a normally distributed random error.
5. If $j < m$, then go to step 2.

This algorithm can be presented in the following recursive form: $\delta d_j = \sum\limits_{i=1}^{j-1} \mu_i^j \nu^i + \nu^j$, where

$$\mu_i^j = a_i^j + \sum_{k=1}^{j-i-1} a_{i+k}^j \mu_i^{i+k}, \quad a_i^j = -\left(\sum_{\{\lambda\}} \frac{\partial T_j}{\partial d_i}\frac{\partial T_j}{\partial d_j}\right) \Bigg/ \sum_{\{\lambda\}} \left(\frac{\partial T_j}{\partial d_j}\right)^2.$$

4. Evaluation of the strength of thickness errors correlation. In [16] the computational manufacturing experiments are applied to the investigation of the error self-compensation effect associated with direct BBM of optical coating production. In this section we consider one of the coating designs from [16] for which the existence of a strong error self-compensation effect was predicted. This is the so-called non-polarizing edge filter (NPEF).

The discussed NPEF has 50 layers with alternating refractive indices of 2.35 for odd layers and 1.45 for even layers. The count of layers starts from the substrate on which coating is deposited. The substrate is the standard glass with refractive index 1.52. Layer thicknesses are shown in Fig. 1a. The coating is intended for using at oblique light incidence of 45 degrees and must have close reflectance properties for the s- and p-polarized light. For the both states of polarization, it must provide the low reflectance in the spectral region from 900 nm to 990 nm and the high reflectance in the spectral region from 1010 nm to 1100 nm. The coating reflectances for the s- and p-polarized light are shown in Fig. 1b. Target reflectance values are marked in this figure by crosses. Figure 1c shows errors in layer thicknesses that were obtained in the course of one of the computational manufacturing experiments described in [16]. The reflectances of the perturbed coating with these errors are shown in Fig. 1d.

In [16] the computational manufacturing experiments were performed with direct BBM in the spectral region from 400 nm to 900 nm. The thickness errors shown in Fig. 1c are correlated by this monitoring procedure. The presence of a very strong error self-compensation effect was demonstrated by the comparison of Fig. 1d with the figures presenting s- and p-reflectances of perturbed designs in the case of non-correlated thickness errors. It was shown that, even in the case of such errors with essentially smaller levels of thickness errors in individual layer thicknesses, the spectral properties of NPEF were totally destroyed.

We first check estimate (10) using the error vector presented in Fig. 1c. This estimate gives that, for the presented vector, the correlation strength $\alpha = 0.0058$, i.e., it gives a value much less than 1. To demonstrate that this is indeed a very small value, we performed experiments with one million randomly generated non-correlated error vectors. Figure 2a presents the probability density for the correlation strength α calculated using these vectors. The intervals for calculating the probability density have the width of 0.0001 along the α-axis. The mean of α is equal to 0.9993; in other words, this mean value is very close to 1, which corresponds to the fact that the average value of the square norm $\|W\Delta\|^2$ for one million randomly generated random vectors must be close to the mean value of this square norm on a sphere of unit radius (see Eqs. (9) and (10)).

In Fig. 2a the red curve shows the approximation of the calculated probability density function by a log-normal distribution. The point of maximum of the log-normal probability density function is shifted to the left of 1 because of the asymmetry of this distribution, but the mean of α is equal to 0.996487.

It is worth noting that, in one million experiments with non-correlated error vectors, the probability of getting α smaller than 0.1 is only 0.000333. This is clearly seen in Fig. 2b that shows the left part of the probability density function for α from 0 to 0.2. On the contrary, the computational manufacturing experiments with direct BBM always demonstrate a strong correlation of thickness errors. Among a hundred such experiments, the error vectors gave α greater than 0.1 in only four cases. Figure 3a shows the histogram of the obtained α in these experiments.

It can be seen from Fig. 3a that the correlation of thickness errors by direct BBM gives a specific distribution of α that resembles the shape of the log-normal distribution in Fig. 2a. Due to the correlation of thickness errors,

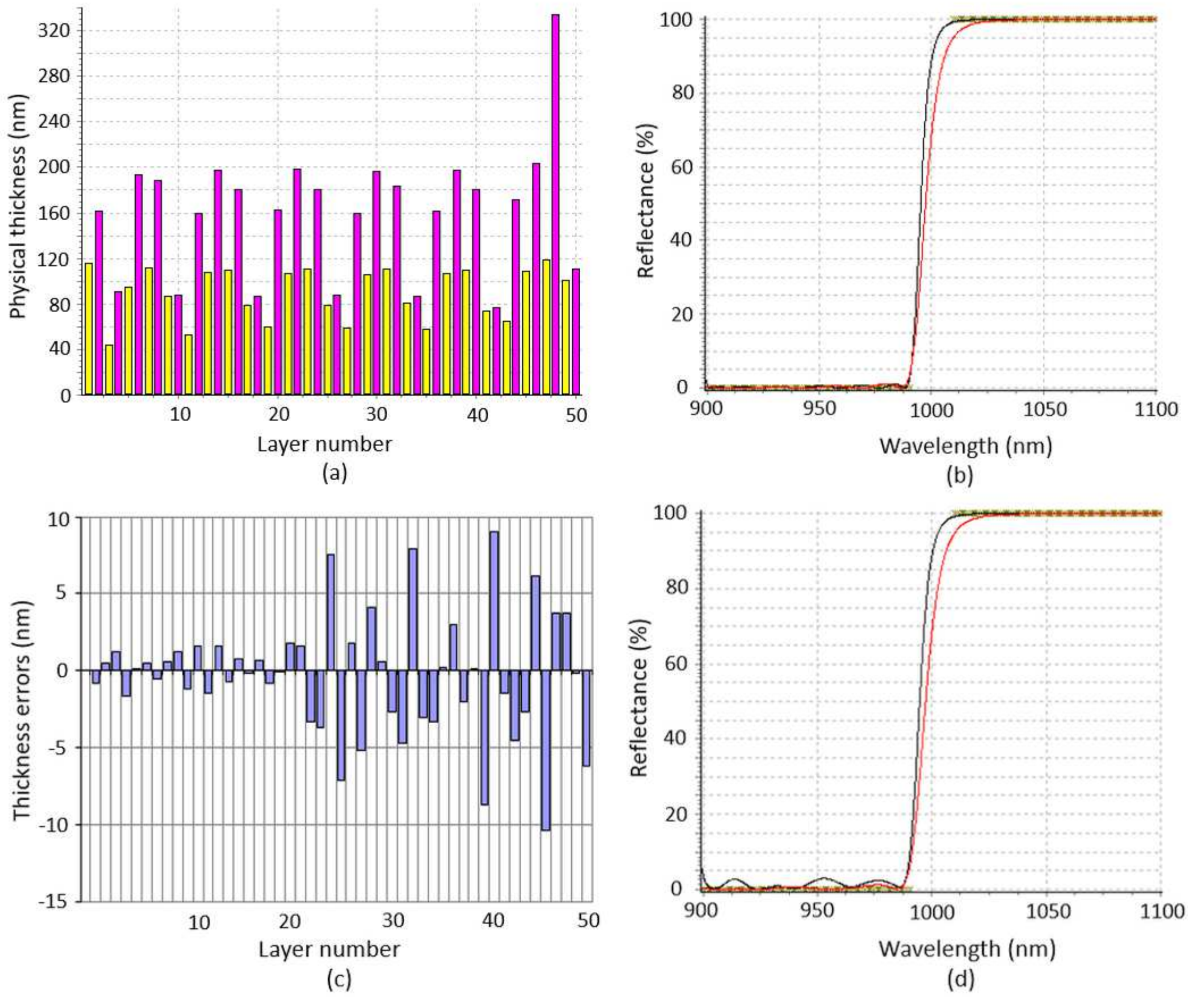

Fig. 1. Layer thicknesses of the 50-layer non-polarizing edge filter (a), s- and p-reflectances of the unperturbed filter (b), errors in layer thicknesses obtained in the course of computational manufacturing experiment (c), s- and p-reflectances of the perturbed filter (d)

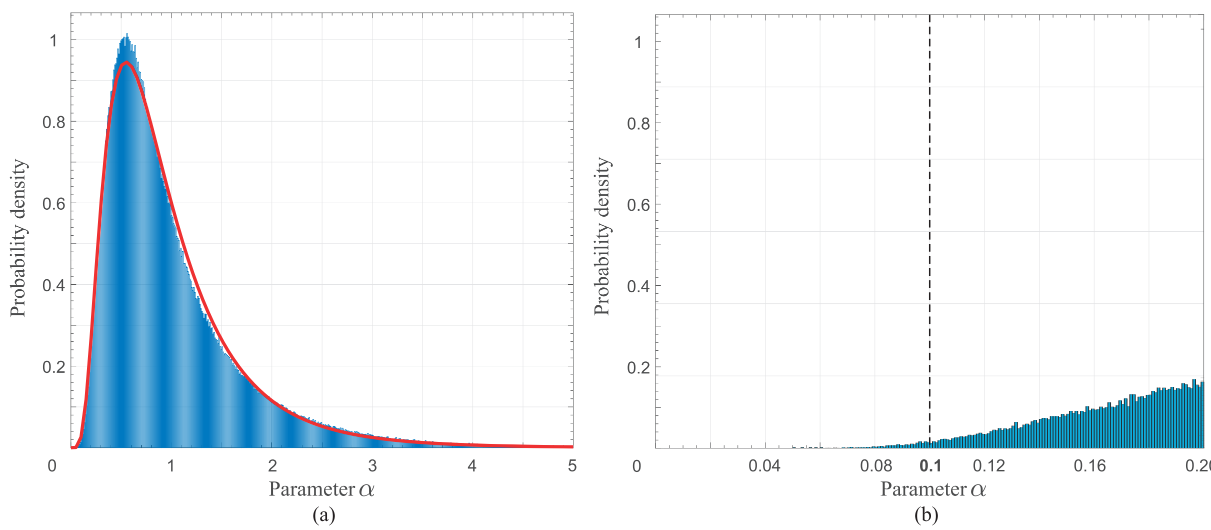

Fig. 2. Probability density for the correlation strength α calculated based on 1 000 000 tests with non-correlated error vectors; red curve shows the approximation of the calculated distribution by the log-normal probability density function (a), the part of the probability density function for the interval α from 0 to 0.2 (b)

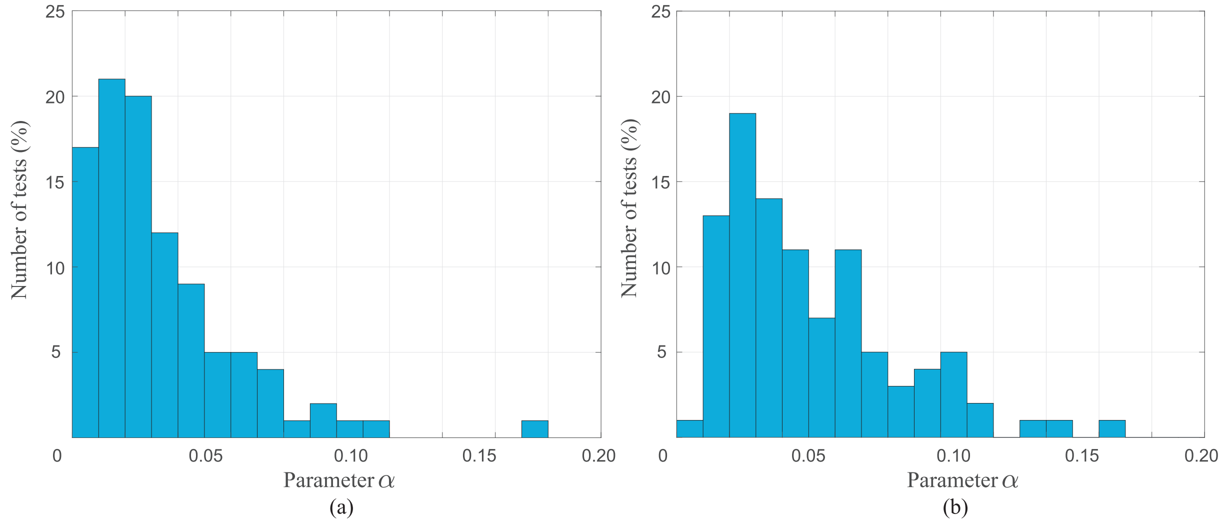

Fig. 3. Histograms showing the numbers of tests giving α in the intervals with 0.01 width: results based on 100 computational manufacturing experiments (a); results based on 100 experiments with the simplified thickness errors simulator (b)

the peak value of this distribution is shifted to the much smaller α value as compared to fig. 2a. It is interesting to analyze this distribution in more detail. Depending on the total number of coating layers, it is possible to perform only dozens or maybe a few hundreds of computational manufacturing experiments in a reasonable time. The detailed investigation of the distribution of α requires generating much more error vectors. For the generation of a significantly larger number of error vectors, we use the simplified thickness errors simulator introduced in Section 3.

Figure 3b shows a histogram similar to that presented in Fig. 3a, but obtained based on 100 experiments with the simplified thickness errors simulator. As one should expect, the histograms in Figs. 3a and 3b are not identical. However, these histograms are qualitatively close. Both these histograms present the α values that are located in the same range of α that is much to the left from the main range of α values in Fig. 2a. Thus, the simplified simulator adequately represents both the random nature of error vectors and the correlation of thickness errors by direct BBM. Figure 4 illustrates the results of one million experiments with this simulator.

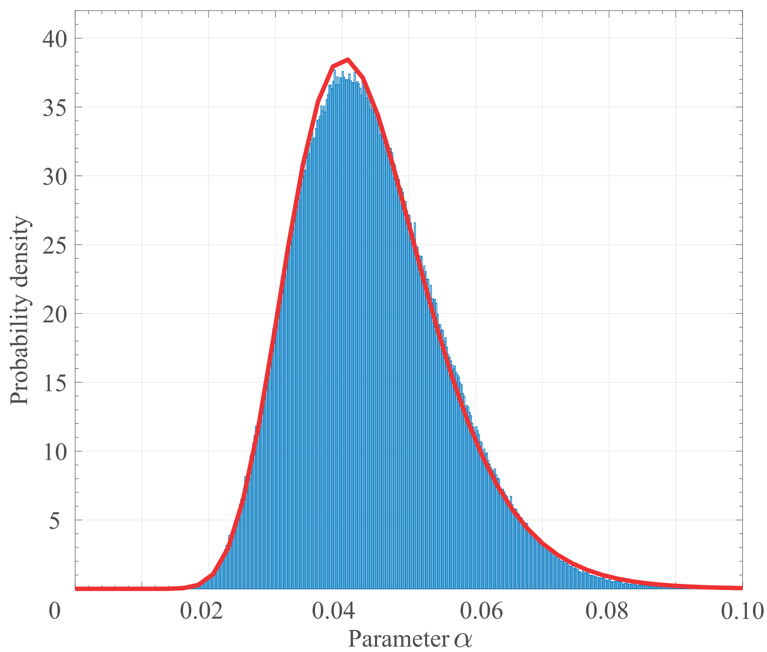

Fig. 4. Probability density function for the correlation strength α calculated based on 1 000 000 error vectors generated by the simplified thickness errors simulator and its approximation by the log-normal distribution (red curve)

As in the case of Fig. 2a, the red curve of Fig. 4 shows the approximation of the calculated probability density function by a log-normal distribution. Despite a quite different range of α and a different nature of generated error vectors (now these are correlated error vectors), the log-normal distribution again provides a very good approximation for the distribution of the correlation strength α. We have performed a number of experiments with other types of optical coatings and other spectral ranges of the BBM procedure and in all cases the log-normal distribution was found to be an excellent approximation for the distribution of the correlation strength α. We assume that this reflects some basic properties of the effect of correlation of thickness errors, but this issue requires more careful study in the future.

Now going back to comparing Figs. 2a and 4, it is necessary to emphasize the two most important features in the distribution of the correlation strength α in the case of correlated thickness errors. First, the maximum coordinate of this distribution is much less than 1; second, this maximum is much larger than the analogous value in the case of non-correlated thickness errors. Obviously, the smallness of the maximum coordinate and the large value of this maximum characterize the strength of thickness errors correlation. To estimate the strength of this effect by some numerical values, thus, one can use these two values calculated using the log-normal approximation of the distribution of α found with the help of the simplified thickness errors simulator.

5. Conclusion. The thicknesses of optical coating layers are the parameters specifying the spectral properties of produced optical coatings. There are multiple random factors associated with the deposition process and layer thickness monitoring that cause errors in the thicknesses of produced optical coatings. The error vectors that present errors in all coating layers have a random character, but at the same time the errors in individual coating layers turn to be correlated by the monitoring procedure. The correlation of thickness errors may produce a positive effect known as an error self-compensation effect, and for this reason the investigation of thickness errors correlation is important for a further progress in the optical coatings technology.

In this paper we propose a robust estimate that can be used to predict the expected strength of thickness errors correlation. This estimate is introduced for the case of the so-called direct BBM technique that is currently considered as the main monitoring technique for the production of the most challenging optical coatings. This estimate allows one to calculate the parameter α characterizing a strength of thickness errors correlation for a given vector of thickness errors.

Because of random character of error vectors, a practical application of the introduced estimate requires statistical analysis. We propose a computationally efficient simulator of error vectors that have a random character and is able to adequately represent the correlation of thickness errors by direct BBM.

A practical application of the proposed estimate is demonstrated using the 50-layer optical coating for which a strong correlation of thickness errors was previously reported in connection with the investigation of a positive error self-compensation effect. The introduced simulator of thickness errors allows us to analyze the strength of thickness errors correlation based on one million tests with correlated thickness errors. It is shown that the obtained distribution of the parameter α is approximated by the log-normal distribution and that the maximum coordinate and the maximum value of the log-normal probability density function are the two values that can be used for representing the strength of thickness errors correlation.

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