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OPTICS AND SPECTROSCOPY. LASER PHYSICS

An Error Self-Compensation Mechanism for Deposition of Optical Coatings with Broadband Optical Monitoring[1]

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Abstract—An error self-compensation mechanism is investigated for use during the deposition of optical coatings with broadband optical monitoring. The correlation of thickness errors caused by monitoring procedure is mathematically described. It is shown that this correlation of errors may result in the effect of self-compensation of errors.

Keywords: thin films, optical coatings, optical monitoring.

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INTRODUCTION

Multilayer optical coatings are widely used in modern science and technology applications, as well as in everyday applications. The introduction of new coatings is connected with the progress in the development of computational techniques for their design [1] and with substantial progress in the development of deposition techniques for these coatings [2, 3]. Further extension of applications of optical coatings and improvement of their characteristics significantly depend on increasing the accuracy of monitoring the specified theoretical thicknesses of coating layers during the deposition process. Increasing attention is paid to the production of optical coatings using broadband optical monitoring of layer thicknesses [4]. This is connected with the expectation that broadband optical monitoring might reduce the influence of production errors on the characteristics of a coating.

It is well known that the quality of deposited multilayer optical coatings significantly depends on the method of monitoring deposition. This dependence reveals itself most dramatically during the production of narrowband interference filters, in particular, filters for telecommunication applications. The number of layers of modern WDM–HDWDM filters may easily exceed several hundred and the production of such filters is only possible using turning-point optical monitoring at the central wavelength of a filter [5]. This is connected with the existence of a very strong error self-compensation effect that is provided by this type of monochromatic monitoring [6–8]. The existence of this effect has been known for more than 40 years, but its physical explanation was suggested relatively recently [9].

The first works on the production of optical coatings with broadband optical monitoring of layer thicknesses were published more than 30 years ago [10–12]. It was already noted in these early papers that broadband monitoring provides some type of error self-compensation mechanism. However, this assumption was not investigated theoretically until recently. Some computational experiments that show that the error self-compensation mechanism really exists and depends on the type of optical coating were described in [13]. Recently, a strong error self-compensation mechanism was observed during the broadband optical monitoring of a multilayer laser polarizer [14].

[1]The article was translated by the authors.

In this paper we performed a theoretical investigation of the circumstances under which the error self-compensation effect for optical coating production with broadband optical monitoring is possible. The multilayer polarizer from [14] is used as an example. A basic algorithm for broadband optical monitoring is described in Section 1. In Section 2 specific features of the broadband monitoring of a polarizer are investigated. Final conclusions are presented in the last section.

1. BROADBAND OPTICAL-MONITORING ALGORITHMS

In this paper we assume that the data from broadband optical monitoring are the transmittance data $T^j\left(d_1^{\mathrm{a}},\dots,d_{j-1}^{\mathrm{a}},d_j\right)$ measured on a set of wavelengths $\{\lambda\}$ for normal light incidence. Let us denote the theoretical layer thicknesses of a given coating design as $d_1^{\mathrm{t}},\dots,d_m^{\mathrm{t}}$. The refractive indices of layers are fixed and possible errors in the refractive indices are neglected.

Let $T^j\left(d_1^{\mathrm{t}},\dots,d_j^{\mathrm{t}}\right)$ be the expected transmittance at the end of the deposition of the jth layer. This transmittance is calculated using well-known analytical expressions [15]. All transmittance coefficients T^j considered here depend on the wavelength $\{\lambda\}$, but we omit this dependence in a written form.

During the deposition process all layers are deposited with some error. The actual thicknesses of the previously deposited layers are indicated with the upper index *a*. We consider the transmittance $T^j\left(d_1^{\mathrm{a}},\dots,d_{j-1}^{\mathrm{a}},d_j\right)$ where $d_1^{\mathrm{a}},\dots,d_{j-1}^{\mathrm{a}}$ are the unknown actual thicknesses of the previously deposited layers and d_j is the variable thickness of the jth layer. The measurement data acquired during the deposition of the jth layer is

$$T^{j,\mathrm{meas}}\left(d_j\right)=T^j\left(d_1^a,\dots,d_{j-1}^a,d_j\right)+\delta T_{\mathrm{meas}},$$

where δT_{meas} are errors in measured transmittance data (these errors also depend on the wavelength λ).

For broadband monitoring we introduce the discrepancy function F^j, which estimates the difference between measurement data and expected transmittance at the end of the deposition of the jth layer. The deposition of the jth layer is terminated when the minimum of the discrepancy function is achieved:

$$\begin{aligned}F^j\left(d_j\right)=&\sum_{\lambda}[T^j(d_1^{\mathrm{a}},\dots,d_{j-1}^{\mathrm{a}},d_j)\\&+\delta T_{\mathrm{meas}}-T^j(d_1^{\mathrm{t}},\dots,d_j^{\mathrm{t}})]^2\rightarrow\min.\end{aligned}\tag{1}$$

The sum is calculated for all wavelengths from the monitoring wavelength grid.

The thickness of the jth layer at the minimum of function (1) is

$$d_j=d_j^{\mathrm{t}}+\delta d_j,$$

where d_j^{t} is the expected theoretical thickness of the jth layer and δd_j is the error in the thickness of this layer.

We consider the thickness errors that have been already made during the deposition of previous layers $\delta d_i^{\mathrm{a}}=d_i^{\mathrm{a}}-d_i^t$ $(i=1,\dots,j-1)$. Assuming that all thickness errors are small, equation (1) is written at the minimum as

$$F^j(d_j^{\mathrm{t}}+\delta d_j)=\sum_{\lambda}\left[\sum_{i=1}^{j}\frac{\partial T^j}{\partial d_i}\delta d_i+\delta T_{\mathrm{meas}}\right]^2.\tag{2}$$

We can rewrite the functional (2) as

$$\begin{aligned}F^j(d_j^{\mathrm{t}}+\delta d_j)=&\sum_{i,k=1}^{j}\left[\sum_{\lambda}\left(\frac{\partial T^j}{\partial d_i}\frac{\partial T^j}{\partial d_k}\right)\right]\delta d_i\delta d_k\\&+\sum_{i=1}^{j}\left[\sum_{\lambda}\frac{\partial T^j}{\partial d_i}\delta T_{\mathrm{meas}}\right]\delta d_i+\sum_{\lambda}(\delta T_{\mathrm{meas}})^2.\end{aligned}\tag{3}$$

The last term in (3) doesn't vary during the minimization of the functional. We consider the second term in the right hand side of equation (3). We assume that systematic errors in transmittance data T are absent (in practice this requirement is achieved by continuous re-calibration of the measurement system). In this case the measurement errors δT_{meas} in the transmittance data may be considered random and normally distributed.

At present, broadband measurements of transmittance data T are usually made on large wavelength grids with more than 1000 measurement points. The derivatives $\partial T^j/\partial d_i$ of the transmittance coefficients are smooth functions of the wavelength λ. Taking all these issues into account we can assume that the second term in the right hand part of equation (3) is small compared to the first term. Therefore, we can neglect the second term in the right hand part of this equation and the condition (1) for the termination of the deposition of the jth layer can be treated as the condition of reaching the minimum of the first term in the right hand part of equation (3):

$$\sum_{i,k=1}^{j}\left[\sum_{\lambda}\left(\frac{\partial T^j}{\partial d_i}\frac{\partial T^j}{\partial d_k}\right)\right]\delta d_i\delta d_k\rightarrow\min.\tag{4}$$

We consider the matrix C^j with elements

$$C_{ik}^j=\sum_{\lambda}\left(\frac{\partial T^j}{\partial d_i}\frac{\partial T^j}{\partial d_k}\right).\tag{5}$$

Equation (4) requires achieving the minimum of the quadratic form with this matrix. Introducing the vector

$$D^j = \{\delta d_1^{\mathrm{a}}, \ldots, \delta d_{j-1}^{\mathrm{a}}, \delta d_j\}^{\mathrm{T}},$$

we can write the condition for the minimum of this quadratic form as:

$$(D^j)^{\mathrm{T}} C^j D^j \to \min. \quad (6)$$

Equation (6) describes the mechanism for the correlation of the thickness error made during the deposition of the jth layer with the thickness errors that have been already made during the deposition of previous layers.

Therefore, during broadband optical monitoring all errors in layer thicknesses are correlated. We now attempt to understand in which cases this correlation of thickness errors may result in the effect of self-compensation of errors.

2. SPECIFIC FEATURES OF BROADBAND MONITORING OF A POLARIZER

The polarizer used here as an example was investigated in detail in [14]. The coating consists of 28 layers with high (ZrO_2) and low (SiO_2) refractive indices. The theoretically calculated layer thicknesses of this polarizer are shown in Fig. 1. At the wavelength of 1064 nm and the light incidence angle of 55.6° this polarizer provides high (more than 98%) transmittance for p-polarization and low (less than 0.6%) transmittance for s-polarization. Monitoring of the deposition process is performed at normal light incidence on the wavelength grid $\{\lambda\}$ with 2036 points in the spectral range from 658 to 1172 nm.

The production errors for the discussed polarizer were estimated in [14]. It was shown that with thickness errors at such a level one should expect a total failure of the spectral properties of the polarizer. However, the spectral properties of the produced polarizer were very good. This means that the correlation of thickness errors connected with broadband optical monitoring produces a strong effect of error self-compensation.

We consider equation (6) from the previous Section. We introduce the diagonal matrix V^j, whose elements are eigenvalues of the matrix C^j in decreasing order. Let P^j be a matrix composed of column eigenvectors of matrix C^j, written in the same order as the eigenvalues. We can rewrite the matrix C^j as

$$C^j = P^j V^j (P^j)^{\mathrm{T}},$$

and the above equation (6) as

$$(D^j)^{\mathrm{T}} P^j V^j (P^j)^{\mathrm{T}} D^j \to \min. \quad (7)$$

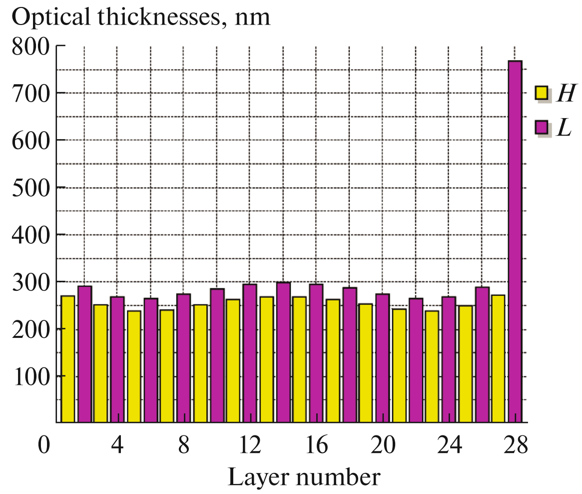

Fig. 1. The optical thicknesses of a 28-layer polarizer.

According to the previous Section, equation (6) specifies the relationship between the thickness error in the jth layer with the thickness errors made in previously deposited layers.

It turns out that for a polarizer all matrices V^j have very specific features, namely, the eigenvalues of C^j matrices decrease very rapidly, while the V^j matrices have only one or two eigenvalues that noticeably differ from zero. As an example, the first three eigenvalues of these matrices for layers five to ten are presented in Table 1.

Consider now the merit function Φ that estimates the quality of the polarizer design. It consists of two partial terms that are responsible for the transmittance in the case of p- and s-polarization (T_p and T_s), respectively:

$$\Phi = \sum_{\Lambda} [T_p(\lambda) - 1]^2 + \sum_{\Lambda} T_s(\lambda)^2. \quad (8)$$

Here, Λ denotes the wavelength grid used to estimate the closeness of transmittance T_p to 1 and T_s to zero. In our case, this wavelength grid consists of 31 wavelength points λ in the vicinity of the working wavelength of the polarizer of 1064 nm.

Table 1. The maximum eigenvalues of matrices C^j for layers five to ten

j	5	6	7	8	9	10
v_1	0.0392	0.0248	0.0595	0.049	0.0838	0.0658
v_2	0.0045	0.0037	0.0093	0.0076	0.0076	0.0109
v_3	0.0018	0.0029	0.0039	0.0036	0.0036	0.0051

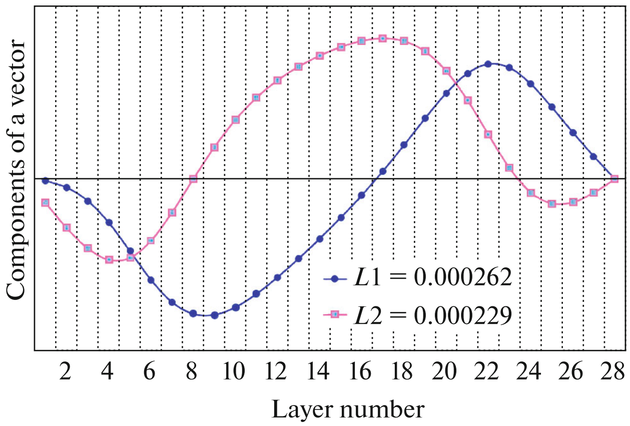

Fig. 2. The eigenvectors that correspond to the first two eigenvalues of the matrix U_p. $L1$, $L2$ are the eigenvalues.

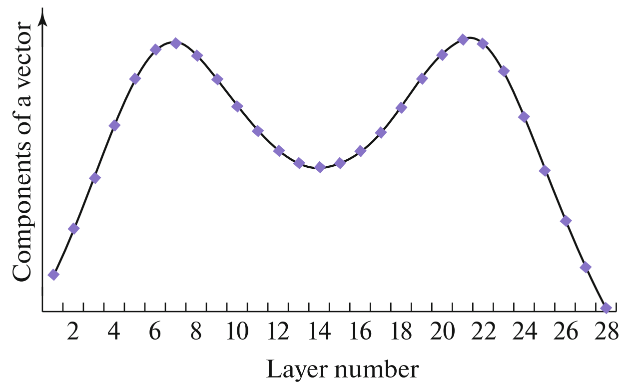

Fig. 3. The eigenvector that corresponds to the first eigenvalue of the matrix U_s.

In (8) both coefficients depend on the layer thicknesses $d_1, \ldots, d_n$ and may be calculated using well-known equations [15]. When solving a design problem, the set of layer thicknesses that provide the minimum of the merit function (8) is found. Therefore, at this minimum the gradient of the merit function is equal to zero and the variation of the merit function is presented as:

$$\delta\Phi = \sum_{i,k=1}^{n} \frac{\partial^2\Phi}{\partial d_i \partial d_k} \delta d_i \delta d_k.$$

Let us introduce the matrix of second-order derivatives

$$A = \frac{\partial^2\Phi}{\partial d_i \partial d_k}$$

and the vector $D = \{d_1, \ldots, d_n\}^{\mathrm{T}}$. Then, we can rewrite the variation of the merit function as

$$\delta\Phi = D^{\mathrm{T}} A D. \qquad (9)$$

By analogy with (7) we can write (9) as

$$\delta\Phi = D^{\mathrm{T}} Q U Q^{\mathrm{T}} D, \qquad (10)$$

where U is a diagonal matrix composed of the eigenvalues of matrix A and the columns of matrix Q are the eigenvectors of matrix A.

Similar equations can be written as well for the partial terms Φ_p and Φ_s in the right-hand side of (8). We denote matrices that are similar to the A and U matrices as $A_{p,s}$ and $U_{p,s}$, and matrices formed by respective eigenvectors as $Q_{p,s}$.

Suppose that in matrices U, U_p, and U_s all eigenvalues are written in decreasing order. It turns out that in our case all of the eigenvalues decrease very rapidly. The eigenvalues are presented in Table 2. In this table they are normalized with respect to the first (maximum) eigenvalue.

Figure 2 presents the eigenvectors that correspond to the first two eigenvalues of matrix A_p. Figure 3 presents the eigenvector that corresponds to the first eigenvalue of matrix A_s.

According to equation (10) for the merit function variation and similar equations for its partial terms, the merit function and its partial terms exhibit the fastest growth in the directions specified by the eigenvectors that correspond to the first largest eigenvalues. It follows that if the vector D, whose components are variations of layer thicknesses, is orthogonal to these eigenvectors, then the variation of the merit function is low. This means that the error self-compensation effect is possible if thickness errors are correlated by the optical monitoring so that the above orthogonality

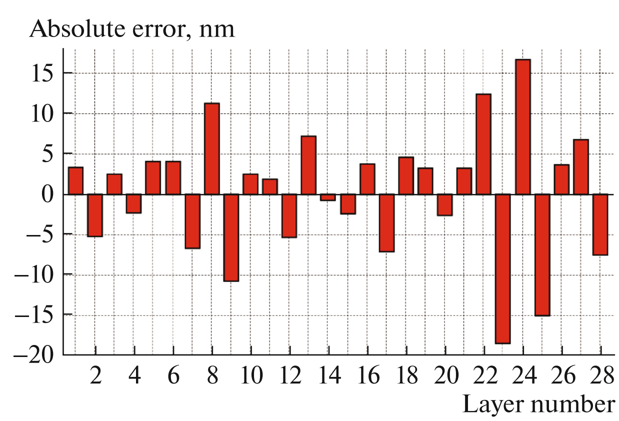

Fig. 4. Polarizer thickness errors.

Table 2. The eigenvalues of matrices A, A_p, and A_s in decreasing order (normalized to the maximum eigenvalue)

Eigenvalue number	A	A_p	A_s
1	1	1	1
2	0.900	0.875	0.072
3	0.453	0.340	0.027
4	0.008	0.006	0.018

Table 3. The angles between the vector of the thickness errors from Fig. 4 and the eigenvectors of matrices A, A_p, and A_s

Eigenvalue number	A	A_p	A_s
1	89.34	89.40	89.48
2	89.23	88.97	89.67
3	88.65	88.82	88.20
4	84.00	84.60	83.10

requirement is fulfilled. We will now check this conclusion using our sample polarizer.

Figure 4 depicts the polarizer thickness errors obtained by solving the inverse problem of finding the layer thicknesses using online broadband optical monitoring of all of the deposition processes. Table 3 presents the angles between the error vector from Fig. 4 and the first four eigenvectors of matrices A, A_p, and A_s.

As one can see, our hypothesis related to the mechanism of error self-compensation effect in confirmed. The requirement of orthogonality is fulfilled for all eigenvalues that noticeably differ from zero (compare with Table 2).

CONCLUSIONS

In this paper the error self-compensation mechanism was investigated for the deposition of optical coatings with broadband optical monitoring. The correlation of thickness errors caused by the optical monitoring procedure was mathematically described. The circumstances under which this correlation of errors may result in the effect of self-compensation of errors were shown. The results were verified and proven using experimental data obtained in the course of the production of a multilayer polarizer.

Further investigations in this area are practically important because they could determine in which cases the broadband optical monitoring of the production of an optical coating provides substantial benefits compared to other modern monitoring techniques.

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