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A new computational method for monochromatic monitoring of optical coatings production

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Abstract: A new method for generating spreadsheets for monochromatic monitoring in the production of optical coatings is presented. The method enables selecting of optimal monitoring strategies for complex optical coatings with a large number of coating layers and an unlimited number of different wavelengths used to monitor their thickness. The proposed approach is oriented to the use of recently developed monochromatic monitoring algorithms. Examples demonstrate its high computational efficiency.

Keywords: optical coatings, monitoring algorithms, monochromatic monitoring.

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Новый вычислительный метод для монохроматического контроля производства оптических покрытий

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Аннотация: Представлен новый метод генерации электронных таблиц для монохроматического мониторинга при производстве оптических покрытий. Метод позволяет выбирать оптимальные стратегии контроля для сложных оптических покрытий с большим количеством слоев и неограниченным числом различных длин волн, используемых для контроля их толщины. Предлагаемый подход ориентирован на использование недавно разработанных алгоритмов монохроматического контроля. Примеры демонстрируют высокую вычислительную эффективность метода.

Ключевые слова: оптические покрытия, алгоритмы контроля, монохроматический контроль.

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1. Introduction. Thin film optical coatings are extremely widely used in most optical and optoelectronic devices. Modern applications require optical coatings with complex spectral properties, the realization of which demands many dozens and even hundreds of layers. The design and production of optical coatings rely on sophisticated mathematical methods [1]. Currently, the main challenge in this field is the development of methods for reliable monitoring of the production of optical coatings with a large number of coating layers.

Optical coatings are produced by depositing successive thin film layers onto substrates in a vacuum deposition chamber. The thicknesses of these layers are determined by solving inverse design problems and must be precisely reproducible during the deposition process. Optical methods for monitoring deposition processes are the primary methods for producing the most complex types of optical coatings [2]. They are based on measuring signal (the transmittance or reflectance of the deposited coating) at short intervals within the vacuum deposition chamber. In this paper, we consider monochromatic monitoring, in which measurements are performed at a wavelength specifically selected for each coating layer.

Monochromatic monitoring has been used to produce optical coatings over forty years. In its original form, called level monitoring [3, 4], it provides signals to terminate layer deposition upon reaching specified

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monitoring signal termination levels. These levels are pre-calculated on the basis of known thicknesses of a theoretical coating design. Unfortunately, accurate control of layer thicknesses using level monitoring is difficult due to a strong cumulative effect of thickness error growth caused by the correlation of these errors during optical monitoring [1]. To minimize this negative effect, modern monochromatic monitoring equipment uses active correction of termination levels based on information about the actual monitoring signal, primarily on the extreme values of this signal recorded during the coating deposition [5–7].

In the context of monitoring with correction of termination levels, the concept of monitoring signal swing is useful [1, pp. 194–196]. It is important for creating monitoring spreadsheets, whose correct specification allows one to utilize all the advantages of modern monitoring equipment in full measure. The monitoring spreadsheet is a table in which each layer is assigned a specific monitoring wavelength and a signal termination level. This paper proposes a new computationally efficient method for creating monitoring spreadsheets for coatings with a large number of layers and almost unlimited number of monitoring wavelength switches between groups of layers, where each such group is monitored at an optimally selected monitoring wavelength. A description of the method is given in Section 2. Examples of the application of this method are given in Section 3. Conclusions are presented in Section 4.

2. Method for creating a monitoring spreadsheet. For certainty, we consider monitoring in transmission mode. The selection of monitoring wavelengths for the coating layers is based on several criteria specified for the dependence of transmittance on the deposited layer thickness. As an example, we will use the criteria discussed in [8] as the most important. Exactly these criteria are specified for the *start amplitude* of the monitoring signal and for its swing value at the beginning and end of layer deposition. It will be seen that the main part of the algorithm does not depend on the set of selected criteria, and the algorithm can be directly used for any other possible combination of the criteria.

In paper [8], the start amplitude of the monitoring signal is the difference between the transmittance level at the beginning of layer deposition (the initial level) and the first transmittance extremum during the layer deposition. Since this difference can be either positive or negative, we will consider its absolute value and denote it as EV value (see Figure 1). This quantity will be called *entry variation*. The extremum of the monitoring signal is not necessarily reached during the layer deposition, and we will extend the definition of the entry variation for such situations. If there is no signal extremum during the layer deposition, then EV is equal to the absolute value of the difference between the transmittance initial level and the termination level (the transmittance level at the end of layer deposition).

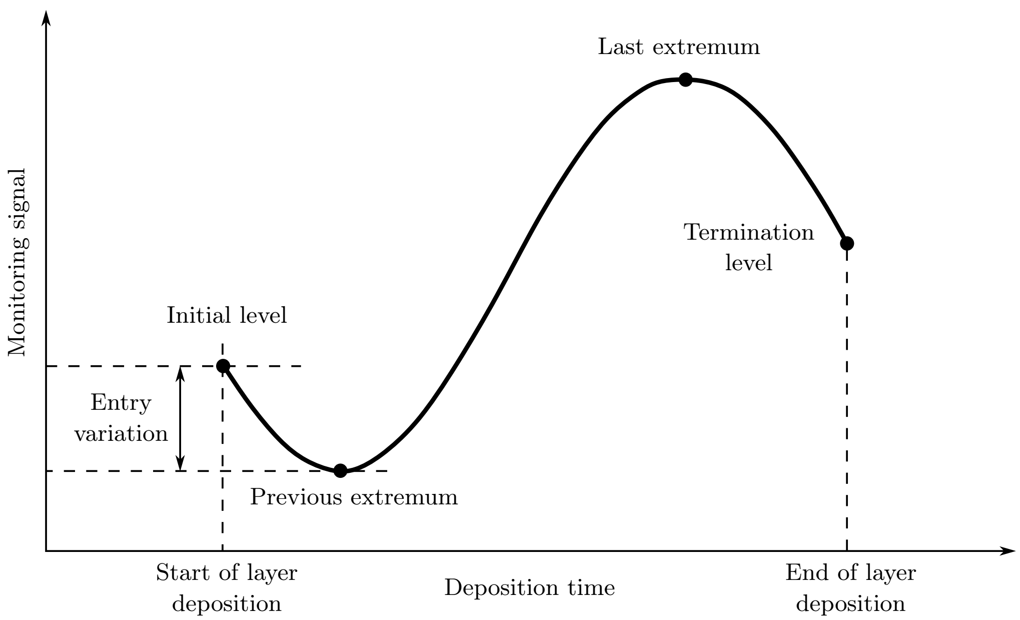

Figure 1. To the introduction of the entry variation EV and swing values

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Along with the EV value, we will consider the initial and final swing values, namely $Swing_{\text{in}}$ and $Swing_{\text{fin}}$. By definition, $Swing_{\text{fin}}$ is related to the termination level $T_{\text{term level}}$ by the formula:

$$Swing_{\text{fin}} = \frac{T_{\text{term level}} - T_{\text{last extr}}}{T_{\text{prev extr}} - T_{\text{last extr}}}. \tag{1}$$

Here $T_{\text{last extr}}$ and $T_{\text{prev extr}}$ are the last two monitoring signal extrema recorded during layer deposition. The quantities included in this formula are shown in Figure 1. The $Swing_{\text{in}}$ value is calculated similarly to the $Swing_{\text{fin}}$ value, but the analog of equation (1) now uses the initial level $T_{\text{initial level}}$ instead of $T_{\text{term level}}$.

We assume that the transmittance is measured as a percentage. Consequently, EV is also measured as a percentage. The same applies to the $Swing_{\text{in}}$ and $Swing_{\text{fin}}$. Figure 1 shows that their values are close to 0% or 100% if the initial or termination levels are close to the maximum or minimum values of the monitoring signal respectively.

Figure 1 illustrates the monitoring of a relatively thick layer, for which two monitoring signal extrema are reached during the deposition process. However, extending the concept of initial and final swing values to thinner layers, when only one extremum or even none of them is reached, causes no difficulties. The expected monitoring signal is pre-calculated using the well-known analytical formulas [1], and in these formulas we can extend the deposition time to the left from the start of the layer deposition. This allows calculating the virtual last and previous monitoring extrema [1].

The use of monochromatic monitoring with termination level correction requires the creation of monitoring spreadsheets with specific requirements to the monitoring signal behavior. Such requirements are particularly important for the monitoring signal at the beginning and end of layer deposition [8]. As an example, we will use the requirements that are considered most significant in [8]. We demand that the entry variation EV exceeds a%, and that the initial and final swing values be within the specified limits. The specific values of a and swing limits in percentage will be set in Section 3.

The requirements for the swing values mean that the monitoring signal cannot begin or end near its extreme values. This ensures that the actual monitoring signal does not lose the extremes present on the theoretical monitoring curve or, conversely, does not create new extremes not present on this curve. The requirement for EV value ensures that variations in the monitoring signal during layer deposition are sufficiently large compared to the inevitable errors in measuring the monitoring signal of the growing layer.

To take these requirements into account, we introduce three partial penalty functions. Firstly, for EV value

$$f_{EV} = \begin{cases} (a - EV)^p, & \text{if } EV < a, \\ 0, & \text{if } EV \geqslant a. \end{cases} \tag{2}$$

Secondly, for $Swing_{\text{fin}}$ value:

$$f_{Swing_{\text{fin}}} = \begin{cases} [w(b - Swing_{\text{fin}})]^p, & \text{if } Swing_{\text{fin}} < b, \\ 0, & \text{if } b \leqslant Swing_{\text{fin}} \leqslant c, \\ [w(Swing_{\text{fin}} - c)]^p, & \text{if } Swing_{\text{fin}} > c. \end{cases} \tag{3}$$

And thirdly for $Swing_{\text{in}}$ similarly to the Equation (3).

The penalty function f is the sum of these partial penalty functions:

$$f = f_{EV} + f_{Swing_{\text{in}}} + f_{Swing_{\text{fin}}}. \tag{4}$$

Note that the penalty function f is zero if all requirements are met. The parameters p and w in (2) and (3) will be specified in Section 3.

Let m be the number of coating layers, and L be the number of wavelength points in the wavelength grid used to select the monitoring wavelengths. When creating a monitoring spreadsheet, one must assign to each coating layer a monitoring wavelength at which the deposition of this layer should be monitored. The penalty function f in (4) depends on the number of the design layer i and the number of the monitoring wavelength l in the specified wavelength grid (l varies from 1 to L). Therefore, we will denote as $f_{i,l}$ the penalty function value for the i-th layer monitored at l-th wavelength. In the algorithm considered, the selection of the monitoring wavelengths is based on minimizing the values of the penalty function $f_{i,l}$. Furthermore, the algorithm also takes into account the requirement to limit the number of wavelength switches during coating deposition. This

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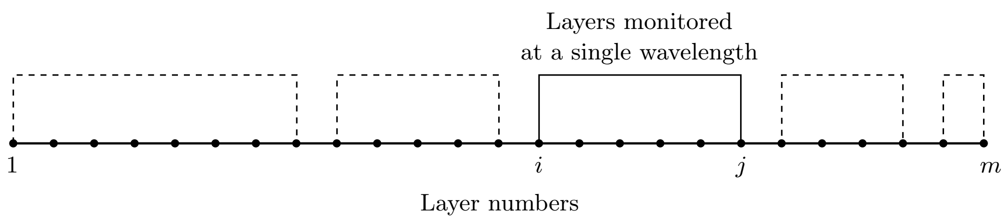

Figure 2. Dividing the design into groups of layers, where each group is monitored at its own wavelength

means that the algorithm generates a specified number of groups of successive design layers, where each group is monitored at its own monitoring wavelength. This is shown schematically in Figure 2.

The algorithm begins by generating a matrix F with the elements $f_{i,l}$ indicated above. This is matrix of size $m \times L$, where L is typically significantly larger than m. The next step is to generate a matrix ψ of size $m \times L$, the elements of which are

$$\psi_{i,l} = \sum_{k=1}^{i} f_{k,l}. \tag{5}$$

When choosing the optimal monitoring wavelength for a sequence of layers, starting from layer i and ending with layer j, we consider the sums of penalty functions for all these layers at different monitoring wavelengths. It is natural to choose the monitoring wavelength so that this sum is minimal. It is easy to see from (5) that these sums are equal to the differences $\psi_{j,l} - \psi_{i-1,l}$. We denote the minimum of this sum by $\varphi_{i,j}$:

$$\varphi_{i,j} = \min_{l}(\psi_{j,l} - \psi_{i-1,l}) \tag{6}$$

and the monitoring wavelength at which this minimum is achieved by $\lambda_{i,j}$.

Now we introduce the table φ with elements $\varphi_{i,j}$ defined by (6). Note that the size of this table is $m \times m$. Since $i \leqslant j$, we only specify its elements on and above the main diagonal. Along with the minimum values defined by (6), this table also stores the wavelengths $\lambda_{i,j}$ at which the minima are reached. This table is the key element of our method. It allows us to select the optimal layer sequences and the optimal monitoring wavelengths for these sequences for any given number of wavelength switches during coating deposition.

In the extreme case, when the monitoring wavelength is the same for all coating layers, the optimal monitoring wavelength is the one listed along with $\varphi_{1,m}$ in the upper right corner of the table. If one or more wavelength switches are set, the optimal combinations are found by enumerating all possible ways to divide the design into groups of layers monitored at the same wavelength. For two monitoring wavelengths, we consider the sums $\varphi_{1,k} + \varphi_{k+1,m}$, where k ranges from 1 to $m-1$. The value of k corresponding to the minimum of this sum indicates the layer number after which the monitoring wavelength should be switched. The monitoring wavelengths for the first and second groups of layers are stored in the corresponding elements of the table φ. For $P > 2$ different monitoring wavelengths, we consider the sums of P penalty terms of the table φ. The process of finding the minimum of these sums can be further accelerated using a standard dynamic programming procedure [9].

3. Examples of monitoring spreadsheets. In the examples of this section, we impose the following requirements on EV, $Swing_{in}$ and $Swing_{fin}$ values. We demand that $EV \geqslant 4\%$ and both swing values be between 10% and 90%. The parameters p and w in Eqs. (2) and (3) are equal to 4 and 0.2, respectively. We consider two filters with significantly different structures. In both cases, the monitoring wavelengths are selected in the spectral range from 400 to 800 nm with a wavelength step of 5 nm.

We consider a 44-layer hot mirror and a 42-layer long pass filter with model high and low refractive indices of their layers equal to 2.35 and 1.45. Substrate refractive index is 1.52. In both cases, the first layer from the substrate is a high index layer.

The theoretical transmittance of the hot mirror and the physical thickness of its layers are shown in Figure 3.

To meet the monitoring requirements formulated at the beginning of this section, we need a relatively large number of wavelength switches. When using three different monitoring wavelengths, the monitoring

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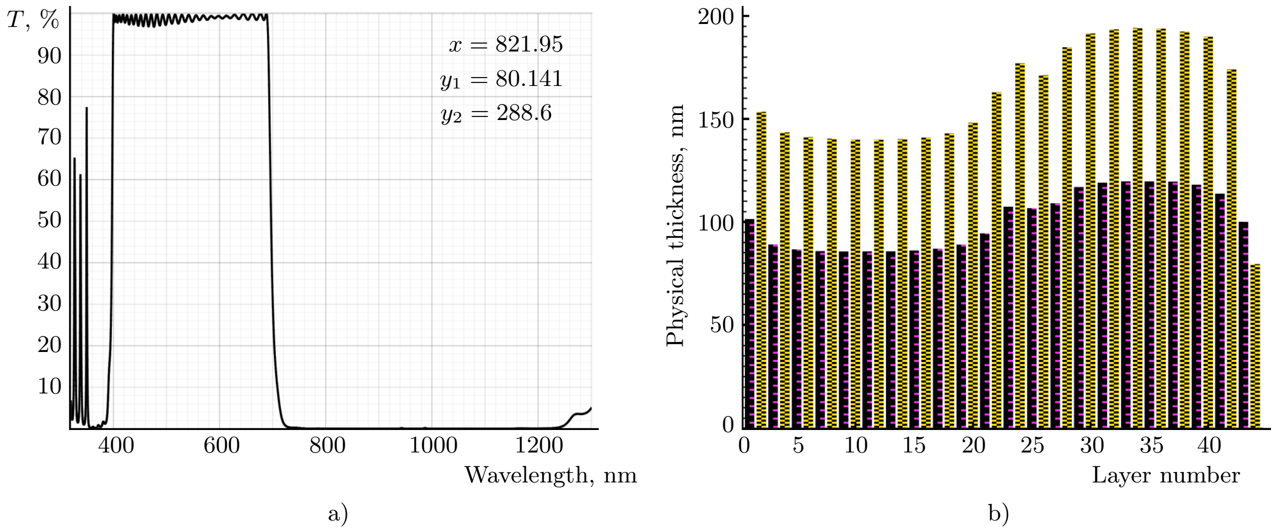

Figure 3. Characteristics of a 44-layer hot mirror: a) theoretical transmittance spectrum; b) layer physical thickness (the dark and light bars represent layers with high and low refractive indices of 2.35 and 1.45 respectively, the substrate refractive index is 1.52)

requirements are violated for eight design layers; when using four wavelengths — for seven layers; and only when using seven different monitoring wavelengths the number of such layers is reduced to three.

Figure 4 shows the monitoring signal corresponding to seven monitoring wave-lengths. The signal is highlighted in pink in the layers where monitoring requirements are violated. These are layers 24, 26, and 32.

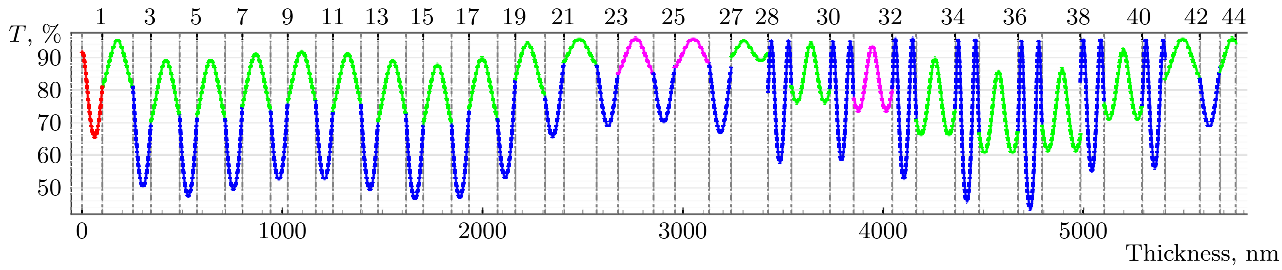

Figure 4. Monitoring signal for a 44-layer hot mirror: layers 1–2 are monitored at 595 nm, layers 3–27 — at 665 nm, layer 28 — at 490 nm, layers 29–38 — at 405 nm, layers 39–41 — at 410 nm, layers 42–43 — at 660 nm, and layer 44 — at 490 nm

For layer 24 — $Swing_{\text{fin}} = 90.3\%$, for layer 26 — $Swing_{\text{in}} = 9.4\%$, and for layer 32 — $EV = 3.9\%$. Clearly, the violations of the formulated requirements should be considered minor.

The theoretical transmittance of the long pass filter and the physical thickness of its layers are shown in Fig. 5.

The layers of this filter are thinner than those of the hot mirror. Therefore, one might expect that more wavelength switches would be needed to meet monitoring requirements. And this is indeed the case. With seven different monitoring wavelengths, there are eight layers where monitoring requirements are violated. Increasing the number of different monitoring wavelengths to eight reduces the number of such layers to five.

Figure 6 shows the monitoring signal corresponding to eight monitoring wavelengths. The signal is highlighted in pink in the layers where monitoring requirements are violated. These are layers 2, 4, 14, 16, and 40.

For layer 2 — $EV = 2.5\%$, for layer 4 — $EV = 3.3\%$, for layer 14 — $Swing_{\text{fin}} = 7\%$, for layer 16 — $Swing_{\text{fin}} = 8.2\%$, and for layer 40 — $Swing_{\text{fin}} = 9.9\%$. Such deviations from the stated requirements are considered acceptable, especially given that further complication of the monitoring strategy does not lead to a significant improvement in the results.

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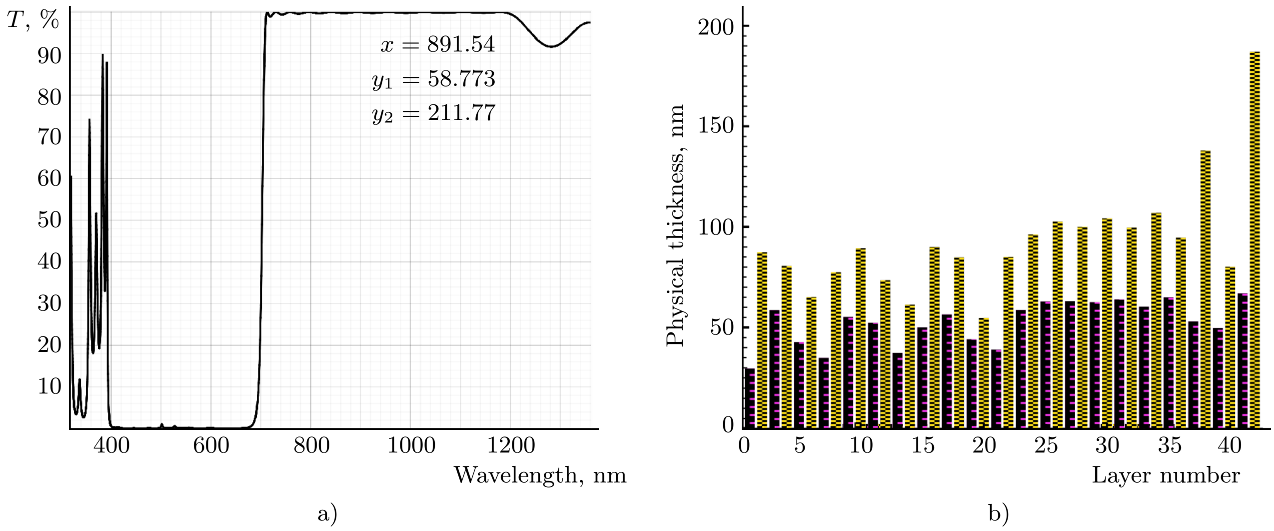

Figure 5. Characteristics of a 42-layer long pass filter: a) theoretical transmittance spectrum; b) layer physical thickness (the dark and light bars represent layers with high and low refractive indices of 2.35 and 1.45 respectively, the substrate refractive index is 1.52)

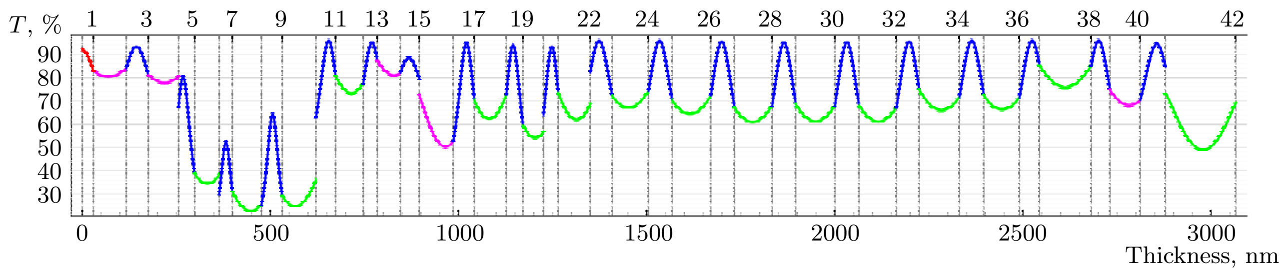

Figure 6. Monitoring signal for a 42-layer long pass filter: layers 1–4 are monitored at 800 nm, layers 5–6 — at 575 nm, layers 7–10 — at 520 nm, layers 11–15 — at 545 nm, layers 16–20 — at 530 nm, layers 21–22 — at 535 nm, layers 23–41 — at 745 nm, and layer 42 — at 705 nm

4. Conclusions. A new method for generating monitoring spreadsheets for coating production with monochromatic monitoring of layer thicknesses is presented. The method is based on assessing the quality of monitoring of successive groups of coating layers at a given monitoring wavelength. To assess this quality, various criteria for selecting a monitoring wavelength can be specified, and a penalty function accounting for those criteria can be introduced. The key element of the algorithm is the construction of a table that stores the minimum values of the penalty function and the optimal monitoring wavelengths for different groups of coating layers. Due to a small dimension of the introduced table, the computational efficiency of the proposed algorithm is high, and it has no limitations on the number of different wavelengths used to monitor the coating production.

The application of the algorithm is demonstrated using the examples of generating monitoring spreadsheets for structurally different multilayer filters. In these examples, we used monitoring wavelength selection criteria that are essential for the reliable application of monochromatic monitoring procedures with on-line correction of the monitoring signal termination levels. In all examples, monitoring spreadsheets containing up to eight different monitoring wavelengths are generated in a fraction of a second on a standard laptop.

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