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Improving the Accuracy of Broad-Band Monitoring of Optical Coating Deposition

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Abstract—A method for improving the accuracy of the broad-band monitoring of the process of depositing optical coatings is proposed. The method is based on determining the actual set of thicknesses of deposited layers in the deposition process. The effectiveness of the proposed approach is demonstrated in a series of model numerical experiments using a simulator of deposition process.

Keywords: multilayer optical coatings, broad-band optical monitoring, spectral characteristics.

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INTRODUCTION

Multilayer optical coatings are widely used in various branches of science and modern technology. The problem of designing an optical coating with the specified spectral properties was successfully solved [1] using a technique for optimizing the coating structure called the method of needle variations, which was proposed in [2]. The most urgent task is to improve the quality of the manufacturing of modern optical coatings. A key problem for solving this task is to improve the reliability of controlling the coating process, because even small deviations of the parameters of deposited coating can lead to significant changes in their spectral characteristics.

Tumerous algorithms developed for controlling the coating deposition process can be divided in two groups: (1) algorithms for determining the thicknesses of already deposited layers, and (2) algorithms for predicting the time when the deposition of the current layer should be terminated. The algorithms of the first group for determining the parameters of deposited multilayer coating will be called characterization algorithms, while the algorithms of the second type will be called monitoring algorithms.

The two most widely used characterization algorithms are called "triangular" and "sequential" (T and S-algorithms) [3–5]. In the case of the T-algorithm, the measurement data obtained for each layer at the end of the process of its deposition are used for determining the thickness of the last deposited layer, as well as for redefining the thicknesses of all the layers deposited previously. In the case of the S-algorithm, the measurement data obtained for each layer at the end of the process of its deposition are used for determining the thickness of only this layer (the thicknesses of the layers deposited earlier are kept constant and equal to the values obtained at the previous steps of the algorithm) [6].

One of the main problems in using the broad-band optical monitoring of the coating process is accumulation of errors of spectral characteristics, which are used in the monitoring algorithms. As was shown in [7, 8], errors in the spectral characteristics can cause a significant negative influence on the solution of the inverse problems of determining the parameters of optical coating. This effect has a negative impact on the accuracy of predicting the moment of terminating the deposition process for the current layer, that, in turn, can lead to a significant difference of the obtained thickness of the layer from its predetermined theoretical value. In this work we consider a method for improving the accuracy of algorithms for monitoring the process of optical coating deposition by redefining the set of layer thicknesses that is used for predicting the time to terminate the deposition process. The effectiveness of this approach is demonstrated in a numerical experiment using a simulator of the coating process.

The structure of this work is as follows. Section 1 gives a brief description of the deposition simulator that is used in numerical experiments. Section 2 describes the features of the effects that decrease the accuracy of estimating the time of terminating the deposition, and describes a method for improving the accuracy of monitoring by redefining the layer thicknesses that are used in the calculations. The main results of the work are outlined in Conclusions section.

1. SIMULATOR OF THE COATING PROCESS

We developed a special simulator of the deposition process of multilayer optical coating to carry out numerical experiments aimed at tasks of controlling the coating process. Similar simulators are widely used in practice [8]. However, in order to work out the algorithms we needed our own special variant, which allows one to analyze all stages of the numerical experiment.

Let us describe the main algorithmic features of this simulator

1. The theoretical design of the optical coating is defined by the set of its layer thicknesses $\{d_j^{\text{theor}}\}$, $j = \overline{1, N}$ (here N is the number of deposited layers; the refraction coefficient of each layer is predefined) and thickness D of the substrate, whose refraction coefficient is described by a known dispersion dependence.

2. Set $j := 1$ (j is the number of the deposited layer).

3. The process of depositing the jth layer of thickness d_j is monitored at a set of discrete time instances $\{t_m\}$, $t_m = \tau_m$, where τ is the time increment of measuring the transmission coefficient. It is assumed that (j – 1) layers with actual thicknesses of $d_1^a, \ldots, d_{j-1}^a$ have been already deposited. These thicknesses differ from the theoretical values $\{d_i^{\text{theor}}\}$, $i = \overline{1, j-1}$ due to both the direct error in the thickness of deposited layers, as well as due to the uncertainties of controlling the deposition process with regard to the minimum of the residual functional for each layer (the corresponding formula for residual functional is given below).

The process of deposition is simulated as follows:

(a) Set $m := 1$ (m is the index of the deposition time instance).

(b) The "true" thickness of the deposited layer $d^a(t_m)$, which is known to the simulator, is calculated according to the relation $d^a(t_m) = d^a(t_{m-1}) + r_m(t_m - t_{m-1})$ (considering that $d_a(t_0 = 0)$, in which $r_m = r + \delta r(t_m)$ (r is the estimated deposition rate, $\delta r(t_m)$ is the stochastic noise with dispersion σ_r^2) with the redefinition of the value of r_m by the closest value from the $[-3\sigma_r; 3\sigma_r]$ segment.

(c) These data form a basis (see, for example, [10]) for calculating the "true" transmission coefficient $T(d_1^a, \ldots, d_{j-1}^a, d^a(t_m), \lambda)$ for each wavelength λ of the light passing through the multilayer coating. The errors that model the "real" transmission coefficient measured in a real experiment are then introduced in the "true" transmission coefficient, including: (1) random noise $\delta T_{\text{meas}}^{\text{random}}(\lambda, t_m)$ (uncorrelated in respect to λ error with dispersion $\sigma_{\text{meas}}^{\text{random }2}$); (2) random shift $\delta T_{\text{meas}}^{\text{fluc}}(t_m)$ (assumed as equal for all λ random fluctuation of the transmission coefficient with dispersion $\sigma_{\text{meas}}^{\text{fluc }2}$); and (3) the systematic error $\delta T_{\text{meas}}^{\text{syst}}$ with dispersion $\sigma_{\text{meas}}^{\text{syst }2}$.

As a result, the expression for the "real" transmission coefficient $\tilde{T}_{\text{meas}|}(d_1^a, \ldots, d_{j-1}^a, d^a(t_m), \lambda, t_m)$ at time t_m takes the following form:

$$\begin{aligned}
&\tilde{T}_{\text{meas}}(d_1^a, \ldots, d_{j-1}^a, d^a(t_m), \lambda, t_m) \\
&= T(d_1^a, \ldots, d_{j-1}^a, d^a(t_m), \lambda, t_m) + \delta T_{\text{meas}}^{\text{random}}(\lambda, t_m) \\
&\quad + \delta T_{\text{meas}}^{\text{fluc}}(t_m) + \delta T_{\text{meas}}^{\text{syst}}.
\end{aligned}$$

(d) The layer thickness $d^{\text{est}}(t_m)$ that is deposited by the given time is estimated:

$$\begin{aligned}
&d^{\text{est}}(t_m) \\
&= \arg\min_{d} \sum_{\{\lambda\}} \left[T(d_1^{\text{theor}}, \ldots, d_{j-1}^{\text{theor}}, d, \lambda) - \underbrace{\left(T(d_1^a, \ldots, d_{j-1}^a, d^a(t_m), \lambda) + \delta T_{\text{meas}}^{\text{random}}(\lambda, t_m) + \delta T_{\text{meas}}^{\text{fluc}}(t_m) + \delta T_{\text{meas}}^{\text{syst}} \right)}_{\tilde{T}_{\text{meas}}(d_1^a, \ldots, d_{j-1}^a, d^a(t_m), \lambda, t_m)} \right]^2.
\end{aligned}$$

If $d_j^{\text{theor}} < d^{\text{est}}(t_m)$, then the process of depositing the jth layer is completed: $d_j^{\text{est}}(t_m) := d^{\text{est}}(t_m)$, $d_j^a(t_m) := d^a(t_m)$, and transition to #4 takes place.

(e) The series of points $(t_i, d^{\text{est}}(t_i)$, $i = \overline{1, m}$ is approximated by the linear dependence $d = r_m^{\text{est}} t + d_m^{\text{shift}}$ and coefficients r_m^{est} and d_m^{shift} are determined. Next, the value of r_m^{est} is redefined by the value that is closest to it from the $[r - 3\sigma_r; r + 3\sigma_r]$ interval.

The expected termination time, which is required for depositing the layer with target thickness d_j^{theor}, is determined:

$$\Delta r = \frac{d_j^{\text{theor}} - (r_m^{\text{est}} t_m + d_m^{\text{shift}})}{r_m^{\text{est}}}.$$

If $\Delta\tau > \tau$, then m is redefined, $m := m + 1$, and transition to #3 takes place. Otherwise, the deposition process is terminated and the resulting thickness d_j^{est} is estimated:

$$d_j^{\mathrm{est}} = \arg\min_{d} \sum_{\{\lambda\}} \Big[T(d_1^{\mathrm{theor}}, \ldots, d_{j-1}^{\mathrm{theor}}, d, \lambda) - \Big(T(d_1^a, \ldots, d_{j-1}^a, d^a(t_m + \Delta\tau), \lambda) + \delta T_{\mathrm{meas}}^{\mathrm{random}}(\lambda, t_m + \Delta\tau) + \delta T_{\mathrm{meas}}^{\mathrm{fluc}}(t_m + \Delta\tau) + \delta T_{\mathrm{meas}}^{\mathrm{syst}} \Big) \Big]^2 .$$

The value of d_j^a is also redefined according to $d_j^a := d^a(t_m + \delta\tau)$ and the formulas given in #3.

4. An additional error δd_j^a with dispersion σ_{add}^2 is introduced into the actual thickness of the deposited layer, $d_j^a := d_j^a + \delta d_j^a$, j is redefined, $j := j + 1$, and transition to #3 takes place.

As a result, the simulator "knows" the following values of the layer thickness: the initial theoretical thickness $\{d_j^{\mathrm{theor}}\}, j = \overline{1, N}$; the "estimated" thickness $\{d_j^{\mathrm{est}}\}, j = \overline{1, N}$, which was determined in accordance with the algorithm for thickness control; and the "true" thickness $\{d_j^a\}, j = \overline{1, N}$, which "is known" only to the simulator.

2. EXPERIMENTS WITH THEORETICAL SERIES OF THICKNESSES OF THE "HOT-MIRROR" TYPE

The main idea of the present work is demonstrated by the example of a computational experiment on depositing a 40-layer optical coating of the hot-mirror type [1]. The experiment was performed with the following set of input parameters: random error $\sigma_{\mathrm{meas}}^{\mathrm{random}} = 1\%$, fluctuation error $\sigma_{\mathrm{meas}}^{\mathrm{fluc}} = 0.5\%$, systematic error $\sigma_{\mathrm{syst}}^{\mathrm{random}} = 0\%$, deposition rate $r = 0.5$ nm/s, the instability of the deposition rate $\sigma_r = 0.2$ nm/s (40%), and the additive error $\sigma_{\mathrm{add}} = 2$ nm.

Figure 1 shows the result of modeling the process of depositing the 28th layer (the total deposition time is $t_{359} + \Delta\tau = 359.6$ s). An abrupt change in $d^{\mathrm{est}}(t_m)$ for $t_m \in [198, 202]$ s is clearly seen. Detailed analysis of a large number of computational experiments on hot-mirror deposition, as well as other types of coatings, shows that a similar effect that is manifested in the abrupt change of d^{est} practically never occurs at a small number j of the deposited layers below 20. However, as the number of deposited layers grows, jumps of d^{est} similar to that in Fig. 1 become increasingly frequent. The errors in the thickness of deposited layers, which is defined as the difference between the real deposited thickness d_j^a and theoretical thickness d_j^{theor}, also increases as the number of deposited layers grows. This effect is well known; it is called the cumulative effect of thickness errors [11]. Our computational experiments showed that both described effects are closely related to each other.

Further analysis of computational experiments showed that the abrupt jumps of d^{est} are related to peculiarities of minimizing the residual functional that is used for determining $d^{\mathrm{est}}(t_m)$ (see #3d of the coating simulator description). As the number of deposited layer increases, the discrepancy between the first and the second terms in square brackets of the expression for this functional, i.e., the discrepancy between $T_m^{\mathrm{est}}(\lambda)$ and $T_m^{\mathrm{meas}}(\lambda)$ (here and below we use the notation $T_m^{\mathrm{est}}(\lambda) \equiv T(d_1^{\mathrm{theor}}, \ldots, d_{j-1}^{\mathrm{theor}}, d^{\mathrm{est}}(t_m), \lambda)$, $T_m^{\mathrm{meas}} \equiv \tilde{T}_{\mathrm{meas}|}(d_1^a, \ldots, d_{j-1}^a, d^a(t_m), \lambda, t_m)$). This discrepancy is clearly seen in Fig. 2, which illustrates the monitoring process at the time close to the position of the jump d^{est} on the time axis). Because in a significant region of the optical control both the dependences are oscillating functions, the condition of the minimum of the residual functional is determined to a significant degree by

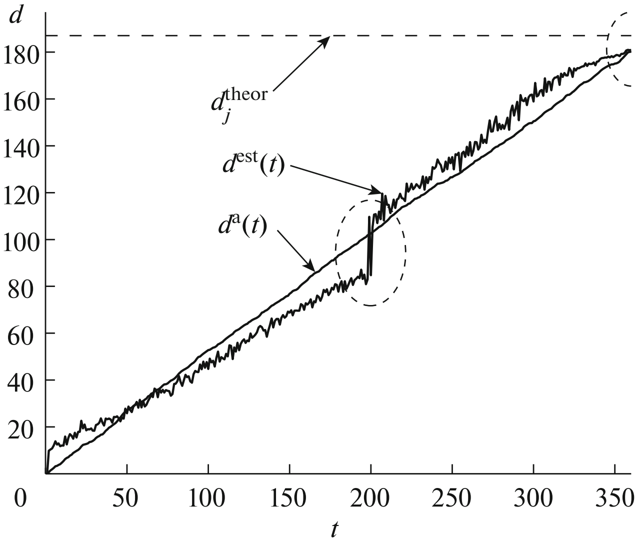

Fig. 1. The result of simulating the deposition of the 28th layer of a 40-layer coating of the hot-mirror type (features of controlling the deposition process are labeled by dashed ovals).

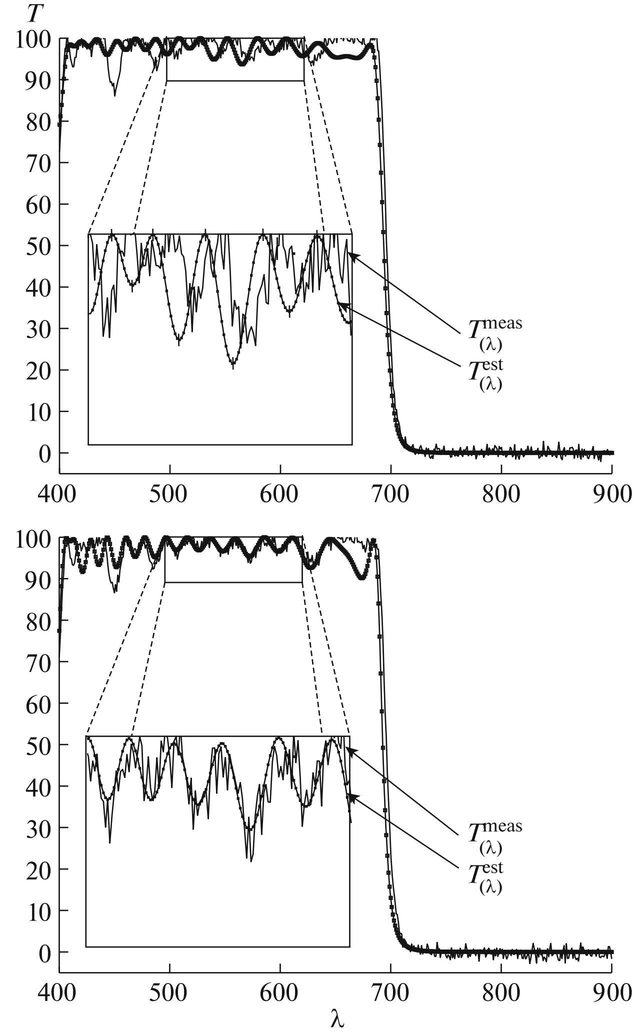

Fig. 2. The "estimated" $T_m^{\text{est}}(\lambda)$ and measured $T_m^{\text{meas}}(\lambda)$ transmission coefficients upon simulating the deposition of the 28th layer at time (upper panel) $t_{197} = 197$ and (lower panel) $t_{198} = 198$.

the proximity of oscillation steps of $T_m^{\text{est}}(\lambda)$ and $T_m^{\text{meas}}(\lambda)$ functions. In turn, the oscillation step of these functions is related to the optical thickness of the coating [12].

Due to the accumulation of errors in the thicknesses of deposited layers, i.e., due to the discrepancy between $d_1^a, \ldots, d_{j-1}^a$ and $d_1^{\text{theor}}, \ldots, d_{j-1}^{\text{theor}}$, the oscillating dependences $T_m^{\text{est}}(\lambda)$ and $T_m^{\text{meas}}(\lambda)$ become increasingly different as the deposited layer number j increases. Computational experiments showed that the abrupt changes of d^{est} are directly due to these discrepancies. Because d^{est} is determined from the condition of the residual functional minimum, at some time instances this function is abruptly changed in such a way as to "adjust" the oscillating dependence $T_m^{\text{est}}(\lambda)$ to the oscillations of the measured dependence $T_m^{\text{meas}}(\lambda)$. This situation is illustrated in the insets to Fig. 2, which show $T_m^{\text{est}}(\lambda)$ and $T_m^{\text{meas}}(\lambda)$ before and after the jump of d^{est}.

As follows from the above, the main reason for the decrease in the accuracy of the layer thickness control as the layer number increases is the growing discrepancy between $T_m^{\text{est}}(\lambda)$ and $T_m^{\text{meas}}(\lambda)$, which in turn is related to the discrepancy of the thicknesses of the deposited layers $d_1^a, \ldots, d_{j-1}^a$ and their theoretical expectations $d_1^{\text{theor}}, \ldots, d_{j-1}^{\text{theor}}$. Therefore, the improvement of the accuracy of controlling the thickness of the deposited layer is related to the possibility of replacing the theoretical layer thicknesses in the residual functional with the $d_1^{\text{ref}}, \ldots, d_{j-1}^{\text{ref}}$ values, which more accurately correspond to the actual values of deposited layer thicknesses $d_1^a, \ldots, d_{j-1}^a$. Such a possibility in fact occurs due to the use of algorithms for defining the parameters of the previously deposited layers in the deposition process. The results presented below were obtained using the T-algorithm, which has proven its usefulness; the definition of the parameters of the deposited layers is performed only once after the deposition of the $\tilde{J}$ layers, where $\tilde{J}$ is a predefined parameter, whose choice is discussed below.

Thus, to improve the accuracy of controlling the layer thickness we propose the following solution. In #3d of the simulator algorithm, instead of minimizing the functional

$$\sum_{\{\lambda\}}\Big[T(d_1^{\text{theor}},\ldots,d_{j-1}^{\text{theor}},d,\lambda) - \tilde{T}_{\text{meas}}(d_1^a,\ldots,d_{j-1}^a,d^a(t_m),\lambda,t_m)\Big]^2,$$

we propose to minimize the following functional:

$$\sum_{\{\lambda\}}\Big[T(d_1^{\text{ref}},\ldots,d_{\tilde{J}}^{\text{ref}},d_{\tilde{J}+1}^{\text{theor}},\ldots,d_{j-1}^{\text{theor}}d,\lambda) - \tilde{T}_{\text{meas}}(d_1^a,\ldots,d_{j-1}^a,d^a(t_m),\lambda,t_m)\Big]^2,$$

in which $\tilde{J}$ values of the theoretical thickness $\{d_j^{\text{theor}}\}$, $j = \overline{1,\tilde{J}}$ are redefined using the T-algorithm after deposition of the $\tilde{J}$th layer.

Figures 3 and 4 shows the calculation results obtained following the refinement of the layer thicknesses after simulating the deposition of 25th layer.

The number $\tilde{J} = 25$ was chosen because numerous computational experiments without redefining the

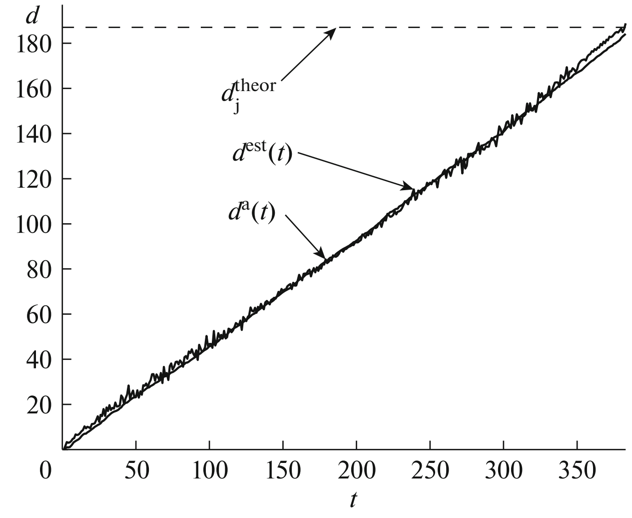

Fig. 3. The result of simulating the deposition process of the 28th layer of a 40-layer coating of the hot-mirror type with redefining the thicknesses of the first 25 layers using the *T*-algorithm.

layer thicknesses have shown that notable growth of cumulative errors occurs after the 25th layer. Similar to Fig. 1, Fig. 3, which is shown for comparison with Fig. 1, demonstrates the estimate of 28th layer thickness in one of the simulations of its deposition. As is seen, abrupt jumps of d^{est} are absent. The same applies to layers with $j > 25$.

Because deposition errors are due to a large number of random factors, the effectiveness of the proposed approach for improving the accuracy of the broad-band control of the deposition process can be evaluated only statistically. In order to obtain such an estimate we carried out two series of numerical experiments in which the layers were deposited without and with redefining the layer thicknesses at $\tilde{J} = 25$. The number of experiments in each series was 10. Figure 4 shows the mean square errors in the thickness of the deposited layers, $\langle d_j^a - d_j^{\text{theor}} \rangle$, calculated based on these experiments. As is seen, due to redefining the thicknesses of the first 25 layers, the accuracy of controlling the thickness of the $j > 25$ layers is improved.

CONCLUSIONS

At present, the broad-band monitoring of the deposition optical coatings is considered as the most promising control method for producing innovative coatings with unique optical properties. However, its wide use in depositing complex coatings with a large number of layers is hampered by the possibility of the cumulative growth of the errors in the layer thickness as the number of deposited layers grows. In the present work using computational experiments to simulate the layer deposition we revealed the main cause of the errors in the algorithms for determining the time when the layer deposition should be terminated and proposed an approach to improve the accuracy of controlling the deposition process by redefining the layer thicknesses which are used in calculations.

The deposition simulator developed for numerical experiments can be used in practice for determining the number of deposited layers after which it is advisable to introduce a layer-thickness correction in the algorithms for determining the termination times of layer deposition that are used by devices of broad-band control.

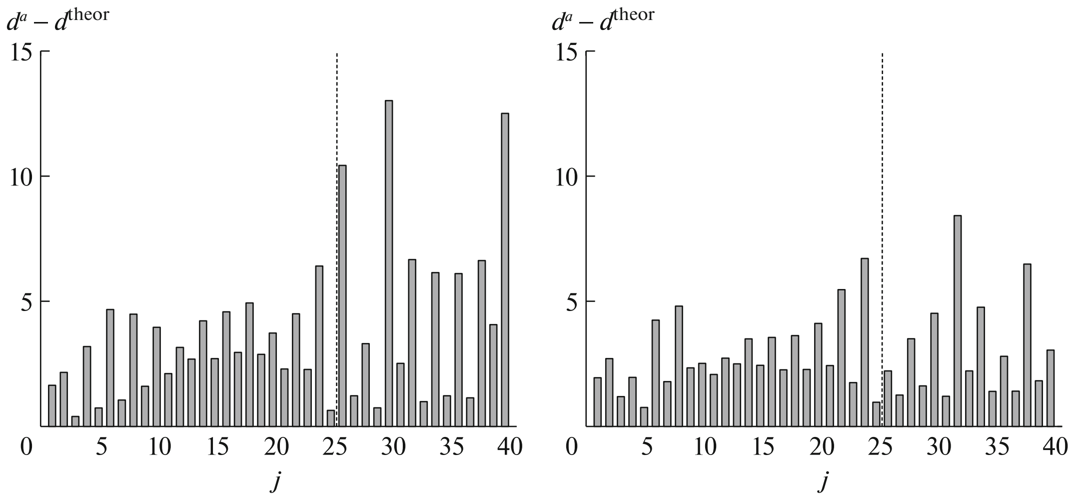

Fig. 4. The mean-square errors $\langle d_j^a - d_j^{\text{theor}} \rangle$ in deposited layers (left diagram) without and (right diagram) with redefining the thicknesses of the first 25 layers using the *T*-algorithm.

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