

## Synthesis of optimal multilayer periodic systems: multicriterial approach and realization of synthesized system

*A.Belyaeva, A.Galuza, S.Kolomiets*

National Technical University "Kharkiv Polytechnical Institute",  
21 Frunze St., 61002 Kharkiv, Ukraine

A novel effective approach to formulation and solving of a multilayer system synthesis problem has been developed. The main characteristics of the system spectrum are used as quality criteria to formulate the multicriteria optimization problem. The preliminary analysis of a specific system has been shown to simplify the optimization procedure essentially and to obtain a unique solution of the problem. A set of examples illustrates the efficiency of the developed approach. Physical reasons for deviations of experimentally realized system from the synthesized one have been formulated.

Развит новый подход к постановке и решению задачи синтеза многослойных систем. Основные характеристики спектра системы использованы в качестве критериев качества, на основе которых сформулирована задача многокритериальной оптимизации. Показано, что предварительный анализ конкретной системы позволяет в ряде случаев существенно упростить задачу оптимизации и получить однозначное ее решение. Эффективность предложенного подхода продемонстрирована на ряде примеров. Сформулированы физические причины возможных отклонений характеристики экспериментально реализованной системы от синтезированной.

Multilayer systems (MS) are the most important elements of modern optoelectronic, optical and other devices. This is connected with the fact that multilayer combination of small quantities of materials provides the systems with unique properties which differ fundamentally from those of individual components. Moreover, varying the geometry and the components, it is possible to obtain the systems with preset properties. The MS quality defines to a great extent the characteristics of devices and constructions. In this connection, in modern editions a lot of attention is given to the problem of MS production with preset properties [1–4]. In the framework of MS development for various applications, there are now the following actual tasks: 1) selection and investigation of new materials; 2) development of new synthesis techniques (the synthesis means selection the optimal MS parameters); 3) development of new quality criteria describing adequately the requirements for

coating physical characteristics; 4) development of new technologies for MS preparation. These tasks should be solved simultaneously to design most effective new multilayer systems. The tasks 2 and 3 are interrelated, namely, the selection of quality criterion influences the synthesis method and vice versa.

In most cases, the synthesis problem is solved according to the following general scheme. At first, a scalar quality criterion is formulated and formalized to take an extreme value for optimal system (the mathematical model of the system to be synthesized is assumed to be known). Usually, mean square deviation of synthesized system characteristics from ideal ones is used as such criterion. At the second stage, the minimum of the obtained quality criterion is searched for in the space of parameters varied. The problem of such approach application to MS synthesis is connected with a number of mathematical difficulties. The



$$\chi = \frac{\varphi(T_{\min} + 0.1\Delta T)}{\varphi(T_{\min} + 0.9\Delta T)}, \quad (2)$$

where  $\Delta T = T_{\max} - T_{\min}$ , while  $\varphi(T_{\min} + 0.1\Delta T)$  and  $\varphi(T_{\min} + 0.9\Delta T)$  are  $\varphi$  values corresponding to transmission on the  $(T_{\min} + 0.1\Delta T)$  and  $(T_{\min} + 0.9\Delta T)$  levels;

4. The width of high reflection range  $\Delta_{\min}$  is defined by the value of spectral range  $\Delta\varphi$  with transmission at its boundaries  $T_{\min} + 0.5\Delta T$  (Fig. 1);

5. Contribution of secondary minima into transmission may be described by integral:

$$I_{trans.} = \frac{1}{\varphi(T_{\max})} \int_{\varphi(T_{\max})}^2 [1 - t(\varphi)]^2 d\varphi. \quad (3)$$

For calculation of MS transmission spectra, the method based on matrix description of thin layer characteristics (Abele method) has been used [8].

Theoretical analysis shows that some values of system parameters may cause not a local minimum at the point  $\varphi = 1$  ( $\lambda = \lambda_0$ ) but a local maximum, which is to be get rid of during synthesis of cut-off filters. For this purpose, the second derivative behavior at  $\lambda_0$  point was analyzed. Positive value of  $T_{\lambda}''(\lambda_0)$  means existence of a minimum at the point  $\lambda_0$  [11], while negative one, a maximum. The  $T_{\lambda}''(\lambda_0)$  analysis resulted in necessity to limit the range of permissible values for multilayer system parameters by the following conditions:

$$\begin{cases} 1 \leq n_L < n_H \leq 5, \\ T_{\lambda}''(\lambda_0, n_H, n_L, m) > 0. \end{cases} \quad (4)$$

The first limitation is naturally imposed on the parameters  $n_H$  and  $n_L$ , because  $n_L$  should be always less than  $n_H$ , it takes into consideration as well the physical limitations on the choice of the materials. The second limitation was obtained as a result of  $T_{\lambda}''(\lambda_0)$  analysis. Fig. 2 shows the region of permissible values of 6-layer system parameters according to the condition (4). The further analysis has shown that as the multiplicity  $m$  increases, the region corresponding to the condition  $T_{\lambda}''(\lambda_0, n_H, n_L, m) > 0$  becomes wider; hence, the requirements to  $n_H$  and  $n_L$  parameters become less strict.

For optimal reflecting filter, the transmission at the point  $\lambda_0$  should be minimal, cutoff sharpness to be maximal, and the

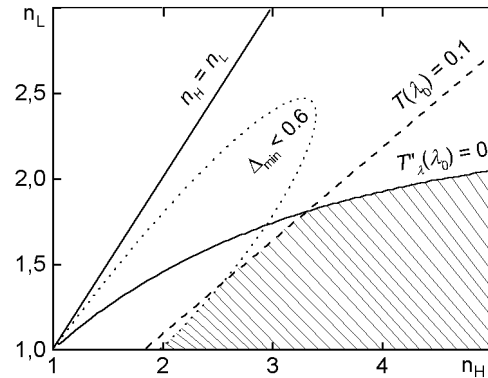


Fig. 2. Diagram  $n_L$  and  $n_H$  values admitted range for system  $[A(LH)^3A]$ : the shaded region demonstrates the range of  $n_L$  and  $n_H$  parameters satisfying the conditions (4)–(6).

number and depths of secondary minima in the operating range (transparency range) to be minimal. At that, the width of the high reflection range should be  $\Delta\varphi \geq 0.5$  (see Fig. 1). It is known from literature that the system main characteristics are defined by MS contrast defined by difference between refraction indices of the layers. In some works [5, 10, 12], such difference is formalized using the parameter  $\Delta n = n_H - n_L$ . However, more detailed analysis carried out in this work has shown that  $\Delta n$  was not a determining parameter for synthesis of optimal periodic systems, but  $n_L$  and  $n_H$  parameters should be considered independently, especially for small  $m$ .

As  $n_H$  increases at fixed  $n_L$ , the characteristics vary in the following way:  $T(\lambda_0)$  tends to zero, while  $\chi$ ,  $\Delta_{\min}$  and  $I_{trans}$  increase, and minimum values  $I_{trans}$  are attained at the minimum  $n_H$  satisfying condition (4). With increasing  $n_L$  at fixed  $n_H$ ,  $T(\lambda_0)$  increases (minimum  $T(\lambda_0)$  is attained at  $n_L = 1$ ),  $\chi$  and  $\Delta_{\min}$  decrease (maximum  $\chi$  values are attained at  $n_L = 1$ ), and  $I_{trans}$  grows (minimum values  $I_{trans}$  are attained at  $n_L = 1$ ). With increasing  $m$  at fixed  $n_H$  and  $n_L$ , the characteristics vary in the following fashion:  $T(\lambda_0)$  trends to zero,  $\chi$  grows, but the range of high reflection becomes narrower, and both the number and the depth of secondary minima increase. So, a contradiction occurs:  $m$  increase results in improvement of some characteristics, while some other ones change for the worse.

The analysis carried out allowed to conclude that to provide optimal MS characteristics, the multiplicity  $m$  should not exceed 3 or 4. Moreover, spectral characteristics can be improved more effectively

using preliminary selection of the materials with further correction by multiplicity.

Qualitative results of the analysis made are listed in Table 1, where sign <+> means improvement, and <-> means worsening of the spectral characteristics at variation of one of three parameters, two other being fixed. It is obvious that variation of system parameters leads to some characteristic improvement, while others are become worsened. Some characteristics change identically (for instance,  $T(\lambda_0)$  and  $\chi$ ). It is worth to note that under increasing the  $n_L$  parameter ( $n_H, m$  being fixed), all the characteristics change for the worse, i.e. for MS synthesis, the parameter  $n_L$  should be chosen as low as possible.

Thus, putting the problem for synthesis of optimal system is complicated by ambiguity of its parameters choice. Moreover, under the synthesis, a simultaneous optimization of several values contradicting to each other is required. Such problem is called the problem of multicriteria optimization and requires the special mathematical methods to be solved.

So, the main spectral characteristics are: transmission minimum in the high reflection range  $T(\lambda_0)$ , cutoff sharpness  $\chi$ , high reflection range width  $\Delta_{min}$ , depths and the number of secondary minima described by  $I_{trans}$  integral. They are determined by the main MS parameters: refractive indices of the layers and multiplicity. It is obvious that for ideal filter, each spectral characteristic should take extreme value (maximum or minimum) on above-mentioned MS parameters. That is why these characteristics may be used to formalize the partial criteria of the system optimality [13]. However, application of all the characteristics for multicriteria optimization problem [14] is not obligatory, because some thereof have similar dependences under variation of the system parameters (Table 1). Of  $\chi$  and  $T(\lambda_0)$  characteristics, only one can be taken for partial criterion, for example,  $\chi$ , while another —  $T(\lambda_0)$  — may be represented as a limitation guaranteeing its definite values:

$$T(\lambda_0) \leq G_1, \tag{5}$$

where  $G_1$  is a certain positive constant which as a rule has a value of the order of 0.1.

The high reflection range width ( $\Delta_{min}$ ) may be presented as well as a limitation, because its extreme values are not critical;

Table 1. Spectral characteristics of reflecting multilayer periodic system depending on MS parameters

Basic parameters	Characteristics			
	$T(\lambda_0)$	$\chi$	$\Delta_{min}$	$I_{trans}$
increasing $n_H, n_L$ , $m$ – fixed	+	+	+	–
increasing $n_L, n_H$ , $m$ – fixed	–	–	–	–
increasing $m, n_H$ , $n_L$ – fixed	+	+	–	–

but it is important that it should be rather wide:

$$\Delta_{min} \geq G_2 \approx \Delta\varphi \approx 0.6, \tag{6}$$

where  $G_2$  is a certain positive constant (Fig. 1).

Fig. 2 shows the  $n_L$  and  $n_H$  values range, satisfying the conditions (4)–(6) for six-layer system  $[A(LH)^3A]$ . Having fixed the minimum value  $n_L = 1$  from the admitted region according to considerations of Section 2, the optimization problem can be reduced to searching for the optimal values of only two parameters:  $n_H$  and  $m$ . As a result, the multicriteria optimization problem becomes the following form

Criteria:

$$\begin{cases} f_1 = N_1 \cdot (1 - \chi) \rightarrow \min, \\ f_2 = N_2 \cdot I_{trans} \rightarrow \min, \end{cases}$$

Limitations:

$$\begin{cases} n_L < n_H \leq 5, \\ n_L = 1, \\ m = 2, 3, \dots, 10 \\ T_{\lambda_0}''(\lambda_0, n_H, n_L, m) > 0, \\ T(\lambda_0) \leq G_1, \\ \Delta_{min} \geq G_2, \end{cases} \tag{7}$$

where  $N_i$  are scale coefficients aimed to reduce all the partial criteria to the [0–1] interval [13].

The generalized criterion is presented as a linear convolution of partial criteria  $f_i$  [13]:

$$F(n_H, m) = \alpha f_1(n_H, m) + (1 - \alpha) f_2(n_H, m), \tag{8}$$

where  $\alpha$  is the weight coefficient.

The Eq.(8) was minimized as follows: for each multiplicity  $m$ , its minimum value was calculated [15] taking into account the limitations (7), among which the minimal one was chosen. This approach is applicable due to discreteness and restrictiveness of a se-

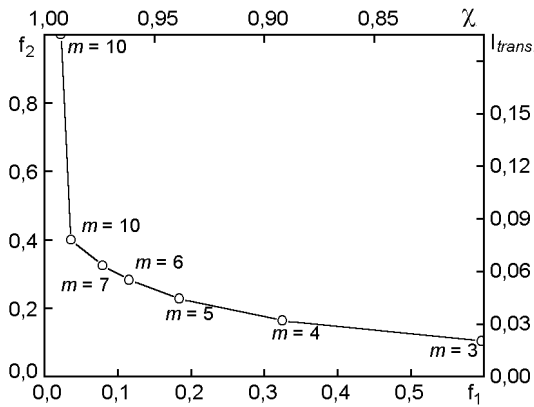


Fig. 3. Pareto set for the problem (7);  $f_1$  criterion characterizes sharpness, and  $f_2$  — secondary extremes.

ries of possible  $m$  values and permits reducing the task to 1D minimization problem. This significantly simplifies the calculation process, and is no doubt among the main merits of the approach proposed.

Detailed behavior analysis of each characteristic and, consequently, the respective criterion, depending on the MS parameters has shown that in the region satisfying the conditions (4) to (6) (Fig. 2), their first derivatives are monotonic functions of the system parameters. Consequently, a linear combination of the partial criteria will have not more than a single extreme. Thus, the preliminary analysis has allowed to guarantee the uniqueness of the solution.

Fig. 3 presents the complete solution of the problem for multilayer system synthesis in multi-criteria formulation (7). The line indicates the set of unimprovable solutions (Pareto set) [16] in the space of criteria. The Pareto set is constructed by minimization of generalized quality criterion for different (generally saying, all the possible) values of weight coefficients. It follows from Fig. 3 that minimum multiplicity values are provided by Pareto set points for which sharpness and secondary extremes possess minimal values ( $f_1$  is maximal). The sharpness is the worst, while the secondary extremes are the best. So, the system designer has a possibility to choose the solution corresponding to his concrete task. A drawback of formulation (7) is impossibility to affect the multiplicity value directly. In some cases, this may restrict application of the problem in formulation (7).

As we shall consider in what follows the systems with minimal number of layers, now we propose another mathematical formulation

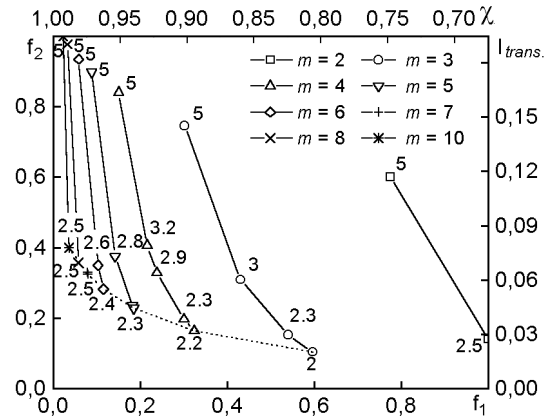


Fig. 4. Pareto set for the problem (9);  $f_1$  criterion characterizes sharpness, and  $f_2$  — secondary extremes; the numbers by the points indicate the  $n_H$  values. Dotted line coincides the points corresponding to solution of (7) task.

of synthesis problem where the possibility to affect the system multiplicity is taken into account using additional partial criterion  $f_3$ . In this case, the problem (7) takes the form:

Criteria:

$$\begin{cases} f_1 = N_1 \cdot (1 - \chi) \rightarrow \min, \\ f_2 = N_2 \cdot I_{trans} \rightarrow \min, \\ f_3 = N_3 \cdot m \rightarrow \min, \end{cases}$$

Limitations:

$$\begin{cases} n_L < n_H \leq 5, \\ n_L = 1, \\ m = 2, 3, \dots, 10, \\ T_{\lambda}''(\lambda_0, n_H, n_L, m) > 0, \\ T_{\min} \leq G_1, \\ \Delta_{\min} \geq G_2, \end{cases} \quad (9)$$

where  $N_i$  are scale coefficients.

The generalized criterion is a linear convolution of partial criteria  $f_i$ :

$$F(n_H, m) = \sum_{i=1}^3 \alpha_i f_i(n_H, m), \quad (10)$$

where  $\alpha_i$  are weight coefficients.

The complete solution of the multilayer system synthesis problem in multicriteria formulation (9) is given as a family of two-dimensional Pareto sets in the  $(f_1 - f_2)$  — space for different multiplicity values  $m$  (Fig. 4). Analysis of Fig. 4 shows that addition of one more criterion  $f_3$  results in a variety of solutions for each multiplicity

(solid lines in the plot). In the present task, variation of weight coefficients with additional criterion  $f_3$  makes it possible to vary the spectrum parameters at fixed system multiplicity. In particular, at small multiplicities, it is possible to vary sharpness in a rather wide range. Also, it follows from Fig. 4 that selecting the high refraction index material gives the opportunity to decrease substantially the secondary extremes with insignificant sharpness drop at fixed multiplicity. The more is  $m$ , the more important the correct choice of the material is, because at  $m \geq 6$ , one can attain more than twice decrease of the secondary extremes without significant sharpness drop (the lines are almost parallel to  $I_{trans.}$ ).

To demonstrate the efficiency of the technique proposed, the problem of designing the interference filter for far IR range was chosen. For such systems, characteristic is the requirement not only to obtain the desired spectrum but to minimize the system multiplicity  $m$  as well [9].

According to the proposed technique, the  $[A(LH)^m A]$  type MS was synthesized [17] basing on the material with the lowest refraction index  $n_L = 1.5$  (polyethylene) which may be used for a layer with low refraction index. At fixed value  $n_L = 1.5$ , the optimization problem is reduced to searching for optimal parameters ( $n_H, m$ ) and takes the following form:

Criteria:

$$\begin{cases} f_1 = N_1 \cdot (1 - \chi) \rightarrow \min, \\ f_2 = N_2 \cdot I_{trans.} \rightarrow \min, \\ f_3 = N_3 \cdot m \rightarrow \min, \end{cases}$$

Limitations:

$$\begin{cases} n_L < n_H \leq 5, \\ n_L = 1.5, \\ m = 2, 3, \dots, 10, \\ T_\lambda''(\lambda_0, n_H, n_L, m) > 0, \\ T(\lambda_0) \leq G_1, \\ \Delta_{\min} \geq G_2. \end{cases} \quad (11)$$

Fig. 5 shows the complete solution of the synthesis problem for such multilayer system in multicriteria formulation (11) as a family of two-dimensional Pareto sets in  $(f_1 - f_2)$  space for different multiplicities  $m$ .

The materials which may be used in MS for far IR as the high refraction index layers combined with polyethylene are KRS-5 ( $n = 2.2$ ), LiF ( $n = 3$ ), and Ge ( $n = 4$ ) [9]. From Fig. 5, it is seen that at the points A

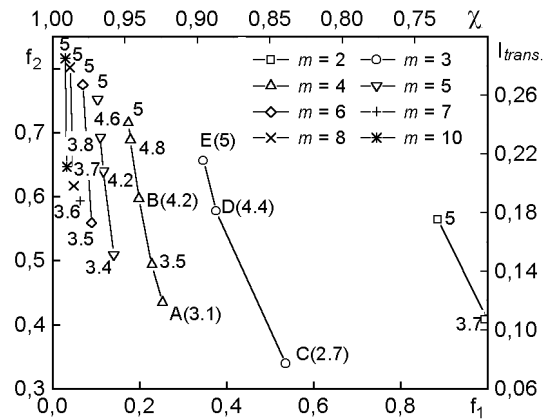


Fig. 5. Pareto set for the problem (11);  $f_1$  criterion characterizes sharpness, and  $f_2$  — secondary extremes; the numbers by the points indicate the  $n_H$  values.

( $n_H = 3.1$ ) and B ( $n_H = 4.2$ ), the values  $n_H$  are most close numerically to  $n$  values of the materials mentioned (LiF and Ge), while there are none of points with  $n_H$  numerically close to the value  $n = 2.2$  (KRS-5).

The characteristics of the system corresponding to point A are:  $T(\lambda_0) = 0.01$ ,  $\chi = 0.9$ ,  $\Delta_{\min} = 0.6$ ,  $I_{trans.} = 0.1$ ; to point B:  $T(\lambda_0) = 0.001$ ,  $\chi = 0.93$ ,  $\Delta_{\min} = 0.75$ ,  $I_{trans.} = 0.18$ . The system corresponding to B point has just a bit different sharpness in comparison with A point, but deeper secondary extremes. Thus, of the systems under consideration, the one corresponding to A point ( $n_H = 3.1$ ) is most preferable. However, from the technological considerations, for far IR it is important to lower the multiplicity of the system synthesized [9, 17].

In the Pareto set, three points correspond to multiplicity  $m = 3$  (Fig. 5): C ( $n_H = 2.7$ ,  $T(\lambda_0) = 0.1$ ,  $\chi = 0.82$ ,  $\Delta_{\min} = 0.61$ ,  $I_{trans.} = 0.07$ ), D ( $n_H = 4.4$ ,  $T(\lambda_0) = 0.006$ ,  $\chi = 0.88$ ,  $\Delta_{\min} = 0.84$ ,  $I_{trans.} = 0.18$ ), and E ( $n_H = 5$ ,  $T(\lambda_0) = 0.002$ ,  $\chi = 0.89$ ,  $\Delta_{\min} = 0.9$ ,  $I_{trans.} = 0.21$ ). It is obvious that the C point has  $n_H$  numerically closer to  $n$  of LiF, and the point D, to that of Ge. The MS corresponding to D point has better spectrum characteristics  $T(\lambda_0)$  and  $\chi$ , but deeper secondary extremes. Of the systems considered, most preferable is the one which has better sharpness and lower background, i.e. the system corresponding to D point. So, in Pareto set, the point has been chosen theoretically which corresponds to the system with minimal multiplicity ( $m = 3$ ), low background ( $T(\lambda_0) = 0.006$ ), good sharpness

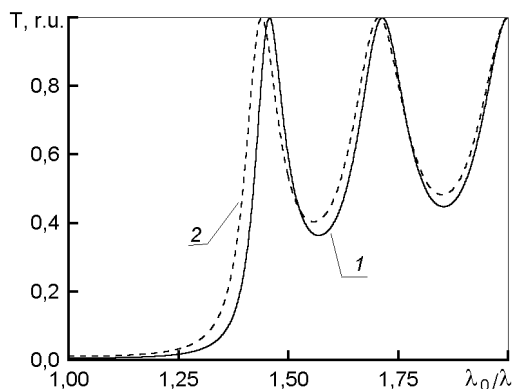


Fig. 6. Transmission spectra of six-layer [A(HL)<sup>3</sup>A] system with parameters  $n_L = 1.5$ ;  $n_H = 4.4$  (1) and  $n_H = 4$  (2).

( $\chi = 0.88$ ) and wide high reflection range ( $\Delta_{min} = 0.84$ ). For the point chosen  $n_H = 4.4$ , that is closest to  $n$  value of Ge ( $n = 4$ ).

In Fig. 6, theoretically calculated transmission spectra of [A(LH)<sup>3</sup>A] MS with parameters  $n_L = 1.5$ ,  $n_H = 4.4$  and  $n_H = 4$  are shown; it is seen that the spectra are essentially the same.

Fig. 7 shows transmission spectra of synthesized (curve 1) and experimentally realized (curve 2) multilayer [A(HL)<sup>3</sup>A] systems with parameters  $m = 3$ ,  $n_L = 1.5$ , and  $n_H = 4$ . It is seen that the produced MS exhibits some quantitative differences as compared to calculated one. These differences may be related to idealization of the model used for synthesis. In this model, the following factors were not taken into consideration: 1) dispersion of refractive indices of the layer materials; 2) absorption in the layers; 3) thickness errors of deposited layers (deviations from quarter-wave rule); 4) scattering due to roughness of the layer interfaces and micro-inhomogeneities in the layer volumes. Curve 3 in Fig. 7 shows that taking into account the factors 2 and 3 provides substantially similar spectra of experimental and synthesized systems.

To conclude, a new technique for synthesis MS based on multicriteria optimization is proposed. Detailed analysis of MS spectrum characteristics as functions of the main parameters is the physical basis for partial criteria choice. The analysis has allowed: 1) to show that no MS parameter selection provides the simultaneous improvement of all the characteristics; 2) to construct the admitted region for the system parameters values; 3) to reduce the number of the fitting parameters; 4) to formulate partial quality criteria; 5) to formalize the

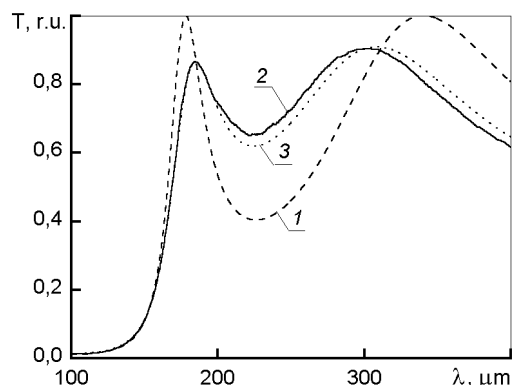


Fig. 7. Transmission spectra of six-layer system with parameters  $n_L = 1.5$ ;  $n_H = 4$ : 1 — synthesized system; 2 — experimentally realized system; 3 — system synthesized taking into account both absorption in L-layers ( $k = 0.01$ ) and random layer thickness deviations.

synthesis problem in multicriteria approach; 6) to simplify optimization procedure and to obtain a single-valued solution of the problem. Using the synthesis problem solution for polyethylene-germanium quarter-wave MS as an example, it was shown how the approach developed may be adopted to synthesis of systems with specific requirements. The polyethylene-germanium system has been synthesized. Physical causes for deviations of experimental characteristics from calculated ones have been considered.

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## **Синтез оптимальних багат шарових періодичних систем: багатокритеріальний підхід та реалізація системи, що синтезована**

*А.І.Беляєва, О.А.Галуза, С.М.Коломієць*

Розвинуто новий підхід до постановки і рішення задачі синтезу багат шарових систем. Основні характеристики спектра системи використовуються як критерії якості, на основі яких сформульовано задачу багатокритеріальної оптимізації. Показано, що попередній аналіз конкретної системи дозволяє у ряді випадків істотно спростити задачу оптимізації і одержати однозначне її рішення. Ефективність запропонованого підходу продемонстровано на ряді прикладів. Сформульовано фізичні причини можливих відхилень характеристики експериментально реалізованої системи від синтезованої.