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Optimization of the parameters of the layer system on the example of the optical structure

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***Abstract* — We have proposed the approach, which can effectively solve the optimization problem of a complex system that has a layered structure. Here the problem is relates to the optics, but the experience of its solution may be extend to other areas of science and technique where are presents a layered structure.**

Keywords — modeling, optimization, the layer system, multidimensional search methods, multilayer interference coating, light transmission

I. INTRODUCTION

Multilayer optical systems' synthesis has gained a considerable development recently. These investigations affect both the development of optics as well as some other fields of technology and science. Optical multilayer coating is used for optical systems in space technology, various optical devices, integral optics, X-ray and neutron spectroscopy, open systems' electrodynamics, and while creating generators and converters of electromagnetic radiation for the equipment control of environmental pollution, etc. The antireflaction optical coating which contains a small number of layers are of particular interest [1]. A Ukrainian physicist Oleksandr Smakula was the first scientist who developed the interference coating in 1935 (he was an employee at Carl Zeiss).

In general the transparent optical coating is a multilayer structure, each layer of which is characterized by two parameters - refractive index of the material from which it is made, and thickness of layer. Mathematical model of light penetration through optical coating is a very complex nonlinear system. The approach proposed in this paper, gives a fairly effective results and lets to create optical systems with predetermined characteristics. Also, this approach may be usefull for other tasks of a different nature, which also have a layered structure.

II. MODELING AND OPTIMIZATION

To estimate the influence of changing interference systems parameters on the resulting transmission the matrix method was used. It based on the determination of a characteristic matrix [2]. The paper uses proposed by F.Abeles in 1950 matrix method for calculating spectral coefficients. This approach remains relevant and widely used so far. Let us assume a multilayer coating consisting of a finite number of homogeneous and isotropic layers.

If the geometrical thickness of a layer is equal to *d*, and refraction coefficient is equal to *n*, the characteristic matrixes of the homogeneous dielectric film have the appearance:

$$M_s(n,d,\lambda)=\begin{Vmatrix}\cos\delta(n,d,\lambda) & -\frac{i}{p}\sin\delta(n,d,\lambda)\\ -ip\sin\delta(n,d,\lambda) & \cos\delta(n,d,\lambda)\end{Vmatrix},\quad (1)$$

where $\delta(n,d,\lambda)=\dfrac{2\pi\cdot n\cdot d\cdot\cos\theta}{\lambda}$ – is the phase thickness of a layer, p=√ε/μ cosδ. In the case when the direction of propagation of radiation coincides with a perpendicular to the interface, δ = 0 and correspondingly $p=n$.

Knowing a characteristic matrix of one layer (1), we can determine a characteristic matrix of *k*-th layer of multilayer systems, as a product of matrixes of each layer:

$$M(\bar{n},\bar{d},\lambda)=M_k(n_k,d_k,\lambda)\cdot M_{k-1}(n_{k-1},d_{k-1},\lambda)\cdots M_2(n_2,d_2,\lambda)\cdot M_1(n_1,d_1,\lambda),\quad (2)$$

where M_j – is a characteristic matrix of j-th layer; $\bar{n}=(n_1,n_2,...,n_{k-1},n_k)$ – is a vector of the values of refraction indices of layers; $\bar{d}=(d_1,d_2,...,d_{k-1},d_k)$ – is a vector of geometrical thicknesses of layers.

From (2) it is easy to find a value of a MLS transmission at the fixed values of $\bar{n}$, $\bar{d}$ and λ:

$$T(\lambda)=1-\left[\left|\frac{n_0(M_{11}(\lambda)+n_S\cdot M_{12}(\lambda))-(n_S\cdot M_{22}(\lambda)+M_{21}(\lambda))}{n_0(M_{11}(\lambda)+n_S\cdot M_{12}(\lambda))+(n_S\cdot M_{22}(\lambda)+M_{21}(\lambda))}\right|\right]^2,\quad (3)$$

where n_0, n_S – are the refraction indices of external environment and substrate accordingly, M_{11}, M_{12}, M_{21}, M_{22} – are the elements of a characteristic matrix M_j.

For the numerical calculation of the transmittance spectra of MLS the objective function is represented as

[3]:

$$\max_{\bar{n},\,\bar{d}} F\left(\bar{n},\bar{d}\right)=\left(\frac{1}{L}\sum_{i=1}^{L}T^{2}\left(\bar{n},\bar{d},\lambda_{(i)}\right)\right)^{1/2}, \tag{4}$$

where L – is a number of a grid points for a spectral interval from λ_1 to λ_2. At the it’s uniform distribution with a step $\Delta\lambda$

$$L=\frac{\lambda_2-\lambda_1}{\Delta\lambda}+1, \tag{5}$$

where λ_1 and λ_2 – are the short-wave and the long-wave boundary accordingly of researched wave spectral region.

In our experience various gradient methods are efficient for a search of the merit function minimum. All the methods of the type imply re-iterated calculations of the merit function and its gradient, i.e., the vector comprised by partial derivatives of the merit function with respect to the layers sought for parameters. These two operations are essential, and so the rate and precision of their fulfillment determine to a considerable degree the calculation potentials of the method [6-10].

Very often multilayer optics synthesis problems are solved success-fully through reiterated optimization of the merit function with series of random starting designs. As a quasioptimal solution, a vector of the coating parameters is taken, which corresponds to the deepest of the obtained minima. Sometimes, it is worthwhile to pick out several quasioptimal solutions, especially, if the minima are about the same depths. The final selection of the best solution can be done on the basis of the results of their practical implementation.

It is difficult to give all-embracing recommendations concerning the starting design choice and algorithm peculiarities for different types of synthesis problems. Let us only note here that good starting designs can be also set in case of wide-band mirrors and polarizer’s synthesis [10-11].

Usually, the steepest descent method predetermines a fast de-crease of the function along the first few directions of one-dimension, minimizations. Then the speed of the decrease slows radically. This is especially evident when the function isolines have a "ravine-like" structure. Experience shows that the merit function isolines in the synthesis problems look exactly like the former. The "ravine-like" pattern of the merit function grows fast as the number of the F-function variables, i.e., the number of the layers increases. The conjugate gradients method allows to manage the ravine-like pattern of the minimized function in a simple and reliable way. The conjugate gradients method differs from the steepest descent one in the fact that a one-dimension minimization is not implemented along the antigradient but rather along some "adjusted" direction obtained with the previous descent direction taken into account [1, 3, 10].

Let us now discuss synthesis problems where the starting design choice is vague, as a rule. Such are the problems of synthesis of antirefrection coatings, neutral beam splitters, multilayer systems featuring non-standard spectral properties. Let us make another remark concerning optimization of multiextremal functions. In principle, there are mathematical methods of their global minimum search. However, a strict employment of these methods which would ensure determining the global minimum is not feasible practically when the number of variables exceeds 1 or 2 because it implies the necessity of tremendous amounts of computer time. Due to this fact, methods are mostly used which, speaking strictly mathematically, cannot guarantee unconditional determining of the global minimum, but they are completely justifiable in solving practical problems. The considerations above, related to a search of quasioptimal solution of the synthesis problems accord with this approach [3].

To optimize very effectively use the Quasi-Newton methods. These methods used to either find local maxima and minima of functions, as an alternative to Newton's method. It is to provide such quasi-Newton methods − Greenstadt's method, the Powell symmetric Broyden (PSB) method, McCormick's method and Pearson's method.

Another effective method is an r-algorithm [3]. r-algorithm is for minimization or maximization of non-smooth functions, which has been somewhat popular despite an unknown convergence rate. This method involves subgradients, but it is distinct from his so-called subgradient method. It can be viewed as a Quasi-Newton method, although it does not satisfy the secant equation. r-algorithm was developed academician Shore at the VM Glushkov Institute of Cybernetics of NAS of Ukraine. In solving the problem of enlightenment optimal coating substrates consisting of a small number of layers, it appears that effective methods are also zero-order - method configuration (Hook-Jeeves) and Rosenbrock’s method. Variable metric methods are less effective.

A problem under consideration for finding optimal parameters for multilayer optical structures may be formulated as a multiextremum task of nonlinear programming. The obtained results have some theoretical interest. Therefore, a scheme for transforming theoretical results into practical ones is proposed, i.e. that leads to finding a multilayer coating that consists of real materials.

This scheme can be implemented in a series of steps.

1. First of all, we should find the best solution for the problem (1-5) using one of the methods for a multidimensional search [3].
2. We should determine materials to the closest received theoretical refractive indices.
3. Defined refractive indexes should be fixed, and thickness optimization is calculated

$$\Omega(\lambda_1,\lambda_2)=\max_{\bar{d}} F(\bar{n},\bar{d})=$$

$$=\max_{\bar{d}}\left(\frac{1}{L}\sum_{i=1}^{L} T^2\left(\bar{n},\bar{d},\lambda_{(i)}\right)\right)^{1/2},$$

considering the restrictions on geometric length

$$50\ nm \le d_j \le 750\ nm.$$

Films with thinner should not be used because of their great sensitivity to technological errors.

In order to prevent the release of the specified variable frame using a standard method, which is the introduction of a new variable *z*, which is related to the type of ratios *d* [3]

$$d_j = d_{j\min} + \left(d_{j\max} - d_{j\min}\right)\sin^2 z_j$$

or

$$d_j = \frac{d_{j\max} z_j^2 + d_{j\min}}{z_j^2 + 1}, \quad j = \overline{1,2m}.$$

This transformation of variables to reduce the problem to the problem of unconditional minimization.

III. RESULTS

Recently in [12] was proposed two components wide band interference filters for visible spectral range. Bat on spectral dependence of transmitivity there are some deviation from ideal curve (Fig. 1, curve 1). In order to improve level of transmitivity in the visible range up to 100% we applied different methods of multidimensional search. During optimization procedure we have found best parameters compare with [12] for antireflecting two component multinary optical coatings.

We used in parallel methods on p processors. In this case the acceleration in time range is possible compare to one processor computer. In linear approximation this acceleration is approximately is as integral part of q=[k/p+1]. On Figure 1 curve 2 is ease seen that optimization parameters which we got are improve spectral dependents of transmitivity compare with results, obtained in [12]. The same can be seen in Figure 2.

In solving any kind of the synthesis problems, it is necessary to" take into account a number of other non-quantitative aspects, including, firstly, the necessary costs of the solution in terms of computer time and labors costs. A waste of many hours in search of an optimal solution is evidently senseless if, on the other hand, we can find within several minutes "an acceptably adequate" solution satisfying all the requirements. All the above causes the following conclusion concerning the merit function optimization: a global optimization is frequently redundant and it is advisable to look for a good feasibility properties of the coating design and a sufficiently thorough local minimum ensuring the required accuracy of the pre-set spectral dependence approximation. Such "quasioptimal" solution is frequently achieved due to a good selection of a starting design for the merit function optimization. The researcher's personal experience is undoubtedly of utmost importance, though a number of common rules can be recommended. This, firstly, concerns, edge filters of various type. It is advisable to use quarter-wave mirrors or some combinations of such mirrors as the first approximation to their design.

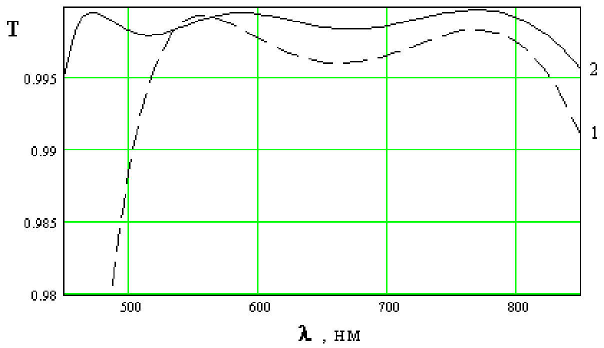


Figure 1. Coefficient of transmittivity for 7 layers two components filters with low (L) and high (H) refractive indexes n_L=1.35, n_H=2.1, substrate n_s=1.52: 1 − optical thicknesses for working wavelength λ_0 are equals 0.06 : 0.02 : 0.35 : 0.02 : 0.07 : 0.42 : 0.21 taken from [12]; 2 − optical thicknesses for working wavelength λ_0 are equals 0.038 : 0.035 : 0.047 : 0.126 : 0.014 : 0.059 : 0.155 after optimization, this work .

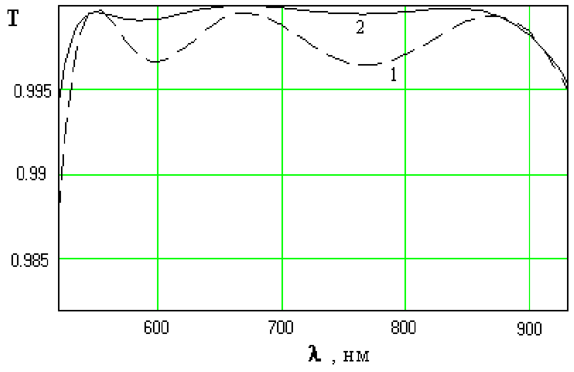
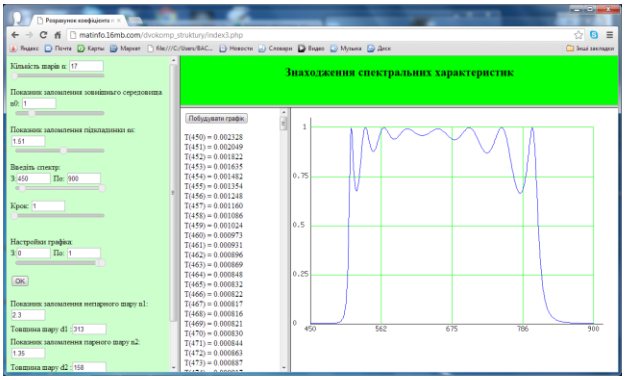


Figure 2. Coefficient of transmittivity for 7 layers two components filters with low (L) and high (H) refractive indexes n_L=1.35, n_H=2.1, substrate n_s=1.52: 1 − optical thicknesses for working wavelength λ_0 are equals .064 : 0.037 : 0.401 : 0.033 : 0.084 : 0.459 : 0.229 taken from [13]; 2 − optical thicknesses for working wavelength λ_0 are equals 0.063 : 0.012 : 0.229 : 0.02 : 0.082 : 0.224 : 0.167 after optimization, this work .

Let us consider the effect of technological errors on the final result. As a rule, the errors are small enough, so it is possible to estimate the influence of the changes in individual parameters by calculating the spectral coefficient derivatives with respect to the corresponding parameter. The first item of the section asserts there are sufficiently simple algorithms allowing to calculate spectral coefficient derivatives very precisely and of low calculation efforts. The possibility of an absolutely precise and fast calculation of spectral coefficients derivatives is of vital importance or design methods of synthesis of multilayer coatings. The major problem in estimating the impact of errors on multilayer coating properties lies in the fact that the concrete values of parameter variations are un known. Usually, we may suggest only some approximate mean values of errors.

The most common and universal approach to determine the technological errors during preparation of optical coatings is Monte Carlo method. But during practical implementation of Monte Carlo method for investigation of optical layered structures, it is necessary to distinguish two issues . The first problem is the need of a large number of experiments. It is known that the statistical error estimates M and σ very slowly decreases inversely proportional to the square root of the number of experiments. The second issue is connected with information about the distribution law of errors during determination of the layers parameters. First of all it is relates to refractive index and thickness of layer, the value and reproducibility of which depends on many parameters during thermal condensation : temperature of substrate; the rate of evaporation and condensation; residual gas pressure in the chamber; the presence or absence of oxidation; cleanliness of materials for evaporation and so on.



Знаходження спектральних характеристик

Кількість шарів n: 17

Показник заломлення зовнішнього середовища n0: 1

Показник заломлення підкладинки ns: 1.51

Введіть спектр: З: 450 По: 900

Крок: 1

Настройки графіка: З: 0 По: 1

Показник заломлення непарного шару n1: 2.3

Товщина шару d1 : 313

Показник заломлення парного шару n2: 1.35

Товщина шару d2 : 158

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T(450) = 0.002328
T(451) = 0.002049
T(452) = 0.001822
T(453) = 0.001635
T(454) = 0.001482
T(455) = 0.001354
T(456) = 0.001248
T(457) = 0.001160
T(458) = 0.001086
T(459) = 0.001024
T(460) = 0.000973
T(461) = 0.000931
T(462) = 0.000896
T(463) = 0.000869
T(464) = 0.000848
T(465) = 0.000832
T(466) = 0.000822
T(467) = 0.000817
T(468) = 0.000816
T(469) = 0.000821
T(470) = 0.000830
T(471) = 0.000844
T(472) = 0.000863
T(473) = 0.000887
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Figure 3. Software interface.

Technology of optical coatings preparation is require reproducible performance and forecasting possible variations in the parameters of layers during preparation. Monte Carlo method allows in the most general terms estimate coating characteristics, investigate the whether of the change (spectral location) and level of light transmission in interference extrema, perform global behavior, predict outcomes due changing of layers characteristics.

A question rises in this connection of how to estimate possible spectral coefficient variations. One of the ways is a multiple reiterated modeling of concrete values of the parameter errors and a subsequent calculation of corresponding spectral coefficients. However, the number of deferent options in modeling the errors is so great, that significant difficulties appear in interpreting the obtained results.

Developed a software that allows you to carry out the necessary calculations associated with optimization of the parameters of multilayer optical structures. Figure 3 shows the interface of this software. Software written in the Java programming language.

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