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NEW METHODS IN COMPUTER-AIDED DESIGN OF MULTILAYERED OPTICAL COATINGS

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Abstract—The synthesis of multilayered optical coatings is considered, including coatings that ensure given spectral characteristics in a wide spectral range; coatings designed for a wide range of angles of incident light; coatings that simultaneously ensure two spectral characteristics (energy coefficients of reflection and transmission); and mirrors with a constant phase shift between the S- and P-components of the reflected field for oblique incident beams. Examples of computer-designed multilayered systems are given.

The last 10 years have seen considerable progress in computer-aided design of multilayered optical coatings and in developing the theoretical fundamentals of analysis and synthesis of layered media. Many achievements have been reflected in recent monographs [1–5] and numerous publications. However better methods are still needed for solving the new multilayer coating problems that arise in various fields of physics and mechanics. Examples of these problems are

- — the development of coatings with specified spectral characteristics in a wide bandwidth;
- — the development of coatings designed to operate over a wide range of angle of incidence, with both converging and diverging light beams;
- — synthesis of coatings subject to two simultaneously specified spectral characteristics (energy coefficients of reflection and transmission);
- — synthesis of coatings with the given energy and phase spectral properties;
- — synthesis of coatings under strict constructional limitations (small number of layers and such);
- — the development of coatings suitable for ultra-short pulses (femtosecond lasers).

This paper presents some new results obtained in handling the aforementioned problems.

1. SYNTHESIS OF METAL–DIELECTRIC COATINGS

Wideband dielectric coatings often evolve as systems with a very large number of layers. This is a technological disadvantage because the quality of such coatings suffers from unavoidable errors in layer thickness in vacuum deposition.

If the coating is expected to be reflective over a wide spectral range, the number of layers in a system may be reduced by using metal interlayers. This method is also of help where it is required to synthesize systems with two specified spectral energy characteristics (or a given absorption coefficient). However, the production of such metal dielectric systems is complicated by the need to take into account the absorptance and dispersive properties of the metals. Grishina and Tikhonravov [6] have developed an efficient design procedure and described a program of synthesis of multilayered optical coatings that allows for the dispersion and absorption of materials. The results of this study are now a basis for a method of synthesis of metal–dielectric coatings with specified spectral properties.

As a first illustrative example we take the synthesis of a wideband rejection filter with a high reflectance in the 0.6–1.0 μm range and a low reflectance at 0.475–0.600 μm wavelengths. A figure of merit for this problem was selected in the form

$$F = \int_{\lambda_1}^{\lambda_2} (R(\lambda) - \hat{R}(\lambda))^2 \, d\lambda$$

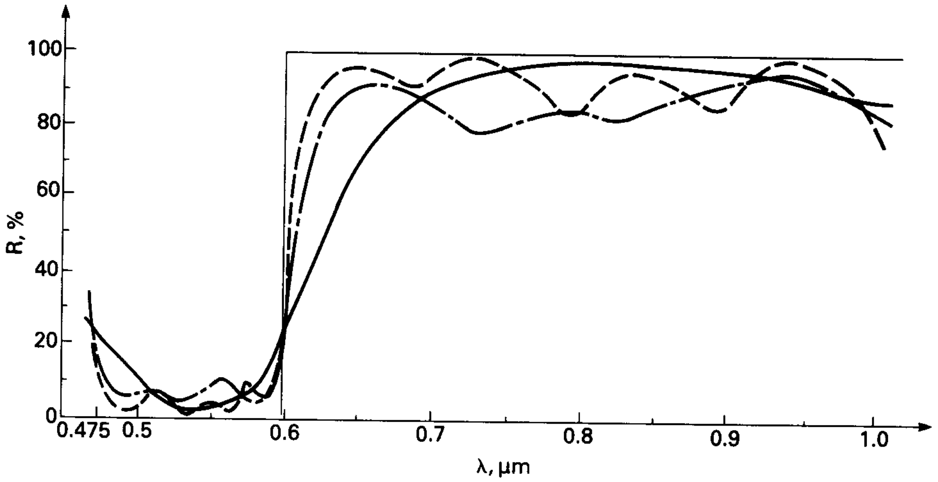

Fig. 1.

where

$\lambda_1 = 0.475$ µm and
$\lambda_2 = 1.0$ µm are boundary wavelengths,
$R(\lambda)$ is the system reflection coefficient,
$\hat{R}(\lambda) = 1$ in the 0.6–1.0 µm range,
$R(\lambda) = 0$ in the 0.475–0.600 µm range.

To test this design in practice a program was developed to synthesize a 3-layered *cover* with a copper interlayer. The first and third layers of the system have $n = 2.30$, the second layer is copper and the refractive index of the substrate is 1.52. For the sake of comparison we present the results of syntheses of dielectric covers having $n = 2.30$ for odd layers and $n_2 = 1.45$ for even layers on the same substrate.

Figure 1 shows the reflection coefficients of three synthesized systems: (a) the 3-layer metal–dielectric system (heavy curve), (b) an 11-layer dielectric system (chain line), (c) a 15-layer dielectric system (dashed curve); and the continuous straight lines represent $R(\lambda)$. The performance of the 3-layer metal–dielectric system is superior in spectral properties to the 11-layer dielectric system, but is somewhat inferior to the 15-layered system. Thus, a metal layer allows for a considerable simplification of the structure and a several-fold reduction of the number of layers.

A second example was to synthesize a coating with a low reflection coefficient and a transmission coefficient in the order of 10% at 0.4–0.7 µm wavelengths. The figure of merit for this case was selected in the form

$$F = \int_{\lambda_1}^{\lambda_2} (T(\lambda) - 0.1)^2 \, d\lambda + \int_{\lambda_1}^{\lambda_2} R^2(\lambda) \, d\lambda$$

where $T(\lambda)$ and $R(\lambda)$ are the energy coefficients of transmission and reflection of the system, $\lambda_1 = 0.4$ µm, and $\lambda_2 = 0.7$ µm.

The material for the metal interlayers was nickel. Figure 2 represents the reflection coefficient (curve 1) and the transmission coefficient (curve 2) for the synthesized 9-layered cover. The refractive indices of the dielectric layers were $n_H = 2.0$ and $n_L = 1.45$; the refractive index of the substrate was $n_1 = 1.52$; and the order of layers from air to substrate was as follows:

$$2(n_L/\mathrm{Ni})/n_H/n_L/n_H/\mathrm{Ni}/n_H.$$

2. SYNTHESIS OF MIRRORS WITH CONSTANT PHASE SHIFT IN OBLIQUELY INCIDENT LIGHT

One of the problems associated with the development of laser physics is concerned with high-reflectance mirrors for obliquely incident light with a constant phase shift between the S- and

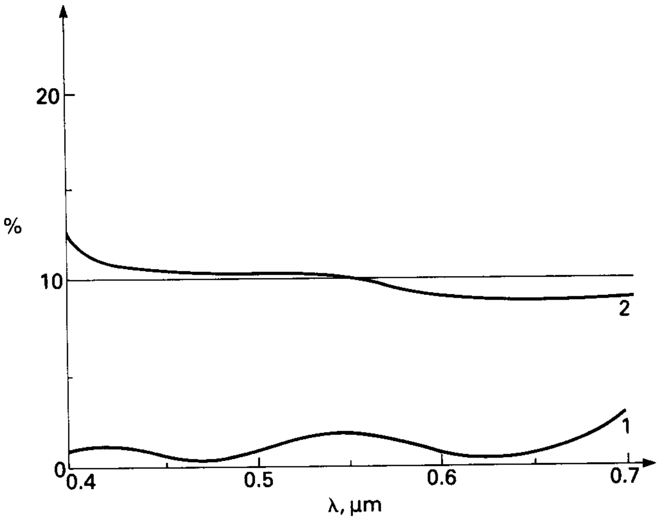

Fig. 2.

P-components of the reflected field. The figure of merit for such a synthesized coating is

$$F=\int_{k_1}^{k_2} w_S(k)(R_S(k)-1)^2\,dk+\int_{k_1}^{k_2} w_P(R_P(k)-1)^2\,dk+\int_{k_1}^{k_2} w(k)(\varphi_S(k)-\varphi_P(k)-\Delta\varphi)^2\,dk$$

where

$k=2\pi/\lambda$ is the wavenumber,
k_1, k_2 is the operative spectral interval,
$w_S(k)$, $w_P(k)$, $w(k)$ are weighting functions,
R_S, R_P are energy reflection coefficients,
φ_S, φ_P are phases of reflection coefficients for S- and P-components,
$\Delta\varphi$ is the required phase difference.

Gradient methods have proved to be inefficient in synthesizing systems having specified phase characteristics. As a rule, they reduce the figure of merit by less than 10–15%. They only correct a little the specified initial approximations of layer thicknesses. To obtain a reliable initial approximation it is usually recommended to make a direct exhaustive search of thicknesses of system layers over the given meshes of values. The mesh should be sufficiently fine—in the order of hundredths of a layer of quarter wavelength thick. High-reflectance systems consist usually of a large number of layers, and therefore an exhaustive search through a separate group of layers would take a prohibitively large amount of computer time.

A way around this problem is offered by the incorporation of the necessary conditions of optimality of the system in the synthesis. The idea of this method has been outlined by Tikhonravov [7] and Baskakov and Tikhonravov [8]. In brief terms it is as follows. The system of differential equations describing the propagation of a wave in the medium is considered along with the adjoint system of differential equations that expresses increments of the performance functional in the local (needle-like) variation of the refractive index (variation of n by Δn on the interval $[\zeta, \zeta+\Delta z]$) in terms of the solutions of these differential systems. The analytical expression for an increment of the performance functional locates a point where variation of the refractive index results in a reduction of the functional.

Assume that the z-axis is directed from the substrate outward. Let 0 and z_0 be the coordinates of the cover boundaries in contact with the substrate and the medium in which the system is immersed, n_1 and n_2 be the refractive indices of alternate layers, and n_0 and n_1 be the refractive indices of the exterior medium and the substrate. If substrate is an absorber, say metal, its refractive index will be a complex quantity, $\tilde{n}_1=n_1+i\psi$. It is convenient to express the amplitude reflection coefficient r_S of the S-component in terms of the admittance X_S, and the amplitude reflection coefficient r_P of the P-component in terms of the impedance X_P, *viz.*

$$r_{S,P} = \frac{v_{S,P} - X_{S,P}(k, z_0)}{v_{S,P} + X_{S,P}(k, z_0)}$$

where $v_S = n_0 \cos\theta_0$, $v_P = (\cos\theta_0)/n_0$, and θ_0 is the angle of incidence.

The equations in X_S and X_P are as follows

$$\begin{aligned} X'_S(z) &= ik(X_S^2(z) + \alpha^2 - n^2(z)) \\ X'_P(z) &= ik(n^2(z)X_P^2(z) - 1 + \alpha^2/n^2(z)) \end{aligned} \tag{1}$$

with $\alpha = n_0 \sin\theta_0$ and the initial conditions

$$X_S(0) = \tilde{n}_1 \cos\theta_l \qquad \text{and} \qquad X_P(0) = (\cos\theta_l)/\tilde{n}_l$$

where θ_l is the angle at which the wave propagates in the substrate.

The energy reflection coefficients and the phases of reflected waves can be expressed in terms of the amplitude reflection coefficients as

$$R_{S,P}(k) = |r_{S,P}(k)|^2,$$

$$\varphi_{S,P} = \arctan\frac{\operatorname{Im}\{r_{S,P}(k)\}}{\operatorname{Re}\{r_{S,P}(k)\}}.$$

The adjoint system of differential equation is in this case

$$\Psi'_{S,P}(z) = 2ikX^*_{S,P}(z)\Psi_{S,P}(z). \tag{2}$$

The initial conditions for the system (2) are given at $z = z_0$ (this system is solved from the external medium to the substrate). The real and imaginary parts of $X_{S,P}$ and $\Psi_{S,P}$ are

$$X_S = x_1 + ix_2, \qquad X_P = x_3 + ix_4,$$

$$\Psi_S = \psi_1 + i\psi_2, \qquad \Psi_P = \psi_3 + i\psi_4.$$

The initial conditions for the system (2) are written in the form

$$\Psi_i(z_0) = -\left.\frac{\partial F}{\partial x_i}\right|_{z=z_0}, \quad i = 1, 2, 3, 4.$$

When the refractive index changes over a small interval $[\zeta, \zeta + \Delta z]$ by Δn, the increment of the performance functional F will be

$$\Delta F = P(\zeta)\Delta z\Delta u + p(\Delta z),$$

where

$$P(\zeta) = -\int_{k_1}^{k_2} k \operatorname{Im}\left(\Psi_S + \frac{\alpha^2}{u^2}\Psi_P - (X_P^*)^2\Psi_P\right)dk,$$

$$u = n^2$$

$$\Delta u = (n + \Delta n)^2 - n^2.$$

For two-component covers, the quantity $|\Delta u|$ is constant, $|\Delta u| = |n_1^2 - n_2^2|$.

In layers with lower refractive index ($\Delta u > 0$), a needle variation leads to a reduction of the functional at points where $P(\zeta) > 0$, whereas in layers with higher refractive index ($\Delta u < 0$) a reduction is observed at points where $P(\zeta) < 0$. The largest variation of the functional will take place at points with the largest magnitude of $P(\zeta)$.

In the synthesis of the coating we look at the solution of systems (1) and (2), compute the value of $P(z)$ and choose a point ζ at which variation of the refractive index results in the largest reduction of the performance functional F. Each local variation of the refractive index at an internal point of a layer is equivalent to a substitution of this layer by three layers, the exterior layers keeping the original refractive index, while the middle layer having a new refractive index over its thickness Δz. A local variation at the interface between two layers simultaneously increases the thickness of

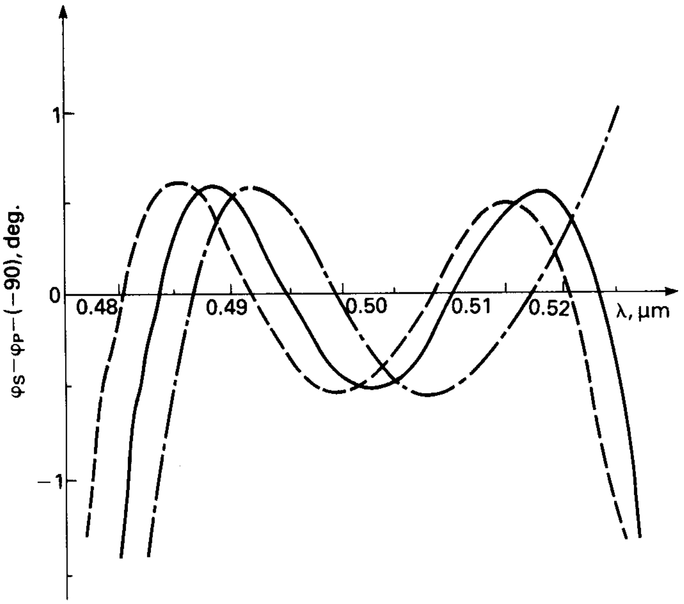

Fig. 3.

one layer and decreases the thickness of the other without altering the total number of layers. If a variation is made at the boundary of a thin layer ($d_j \leqslant \Delta z$), the number of layers decreases.

The method outlined above offers an efficient solution to the problem of a synthesis of mirrors with constant phase shift. By way of example, Fig. 3 shows the deviations of the phase difference from $-90°$ at the angle of incidence $\theta_0 = 45°$ for three synthesized systems. The refractive indices of odd layers (counting from the substrate outward) were 2.30, those of even layers were 1.38 and the refractive index of the S-component for all these systems was $R_S \geqslant 99.9\%$. The first system (curve 1) comprised 34 layers, with substrate refractive index $n_1 = 1.52$, and P-component reflection coefficient $R_P \geqslant 99.8\%$. The second system (curve 2) comprised 31 layers, the reflection coefficient $R_P \geqslant 99.7\%$, and the sum substrate as in the first system. The third system was synthesized on a silver substrate of $\tilde{n}_l = 0.05 + i2.87$. It had 22 layers, and reflection coefficient $R_P \geqslant 99.5\%$.

3. SYNTHESIS OF OPTICAL COVERS WITH SPECTRAL CHARACTERISTICS CLOSE TO SPECIFIED VALUES OVER RANGES OF FREQUENCIES AND ANGLES

Until now methods of synthesis have been designed for optical coatings that operate in some frequency range at normal incidence of light or at a fixed angle of incidence. A more general problem arises when it is required to synthesize a coating that should possess given spectral characteristics not only in a range of frequencies but also in a range of angles. This section describes a method of solving this problem.

We consider absorption-free coating. The spectral characteristics in question are the transmission coefficients of S-polarized light, T_S, of P-polarized light, T_P, and non-polarized light $\hat{T} = (T_S + T_P)/2$. These coefficients are functions of wavenumber, k and angle of incidence, θ.

Practical applications suggest three ways of formulating this synthesis problem.

(1) Synthesize a coating with transmission coefficient for non-polarized light close to the function $\hat{T}(k, \theta)$ specified in the spectral range $[k_1, k_2]$ and in the interval of angles $[\theta_1, \theta_2]$.

(2) The same for polarized light; either $\hat{T}_S(k, \theta)$ or $\hat{T}_P(k, \theta)$ is specified.

(3) Here the two functions $\hat{T}_S(k, \theta)$ and $\hat{T}_P(k, \theta)$ are specified simultaneously. A cover is to be synthesized whose coefficient $T_S(k, \theta)$ is close to $\hat{T}_P(k, \theta)$ and whose coefficient $T_P(k, \theta)$ is close to $\hat{T}_P(k, \theta)$ in the bandwidth $[k_1, k_2]$ and the angle range $[\theta_1, \theta_2]$. The problem is solved by calculus of variations.

To estimate how close the spectral characteristics of a cover lie to those specified we selected

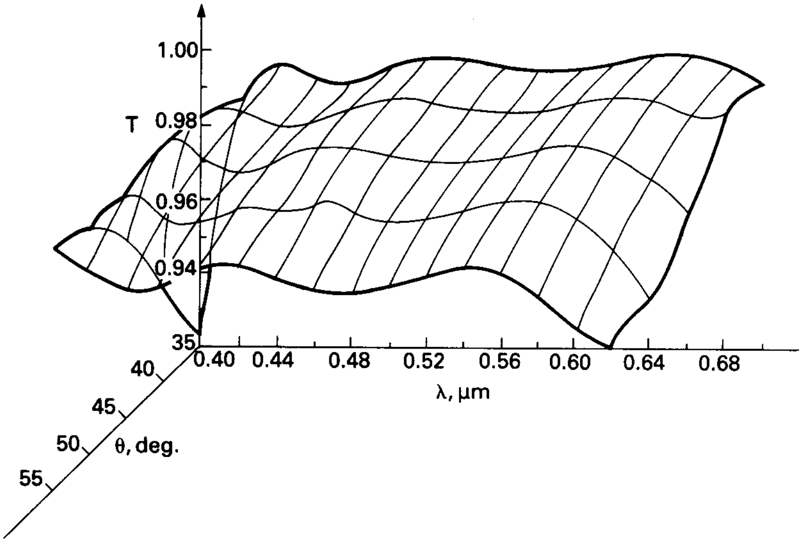

Fig. 4.

the functional

$$F = \int_{k_1}^{k_2} \int_{\theta_1}^{\theta_2} w(k, \theta)[T(k, \theta) - \hat{T}(k, \theta)]^2 \,\mathrm{d}\theta \,\mathrm{d}k \tag{3}$$

for the first formulation, and the functional

$$\begin{aligned} F = \beta & \int_{k_1}^{k_2} \int_{\theta_1}^{\theta_2} w_S(k, \theta)[T_S(k, \theta) - \hat{T}_S(k, \theta)]^2 \,\mathrm{d}\theta \,\mathrm{d}k \\ & + (1 - \beta) \int_{k_1}^{k_2} \int_{\theta_1}^{\theta_2} w_P(k, \theta)[T_P(k, \theta) - \hat{T}_P(k, \theta)]^2 \,\mathrm{d}\theta \,\mathrm{d}k \end{aligned}$$

for the second formulation ($\beta = 0$ or $\beta = 1$) and also for the third formulation ($0 < \beta < 1$). Here, w, w_S and w_P are the weighting functions that allow for different estimations of the accuracy of solutions invarious segments of the spectrum and angle range.

The functionals (3) and (4) allow for the gradient to be written in an explicit analytical form, yielding an efficient algorithm for their computation. Therefore, gradient methods could be used for minimization of the functionals. These methods can form a basis for a universal approach to synthesis of optical coatings.

For all the three formulations of the problem, a software package was written designed for the synthesis of two-component optical coatings. This package proved to be rather efficient, affording syntheses in a range of angles and bandwidth that could be carried out even on a minicomputer. For example, it took only 10 minutes to synthesize an anti-reflecting coating, characterized below, on an SM-1420 minicomputer. The performance specification for this coating stated that it should have $T = 1$ in the visible range (400–700 nm) insensitive to variation of the angle of incidence within 35°–55°. The refractive indices of the external medium (air) was 1.00, and that of the substrate (glass) was 1.52. The layers had $n = 1.45$ and $n = 2.00$.

The initial approximation was an anti-reflecting coating operating at the angle of incidence $\theta = 45°$. This coating cannot be employed at other angles of incidence, for its transmission factor falls to 90% within the above range. The synthesized coating reduces the reflection coefficient down to 1–2% over almost the entire stated frequency range and for all angles of incidence within the interval 35–55°. The spectral characteristics of the design of coating are presented in Fig. 4.

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