A NEW OPTIMIZATION METHODS IN THE SYNTESIS OF MULTILAYER COATING

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ABSTRACT

An efficient method of obtaining the matrices of second derivatives for the synthesis of multilayer coatings, which can also be applied in the case of an absorbent system, is considered. By having the matrix of second derivatives it is possible to employ the rapidly convergent methods of second-order optimization, which in conjunction with the method of acicular variaiations, can be used to develop uniquely efficient software.

I. INTRODUCTION

The antireflection coating is the crucially important technology to obtain high performance in many optoelecronic devices. The designer may be required to provide a coating with many other more complicated properties, including integral quantities such as CİE color coordinates, solar absorptance or emittivity [1]. The parameters that can be used to reach these goals are the number of layers in the multiplayer, the layer thicknesses, and the refractive indices and extinction coefficients of the individual layers and of the surrounding media. Many different methods have been developed for the design of multiplayer coatings [2 - 5].

The method proposed in this paper for computing the Hesse matrix when synthesizing multiplayer coatings permits the use of a wide range of different minimization methods in the software package [3, 5].

II. MATRIX THEORY FOR THE ANALYSIS OF MULTILAYER SYSTEMS

Consider a monochromatic electromagnetic wave with wave number $\kappa\left(\lambda = 2\pi/\kappa\right)$ incident obliquely at an angle θ. Let the refractive index of the substrate be n_0, and let an inhomogeneous multiplayer system of thickness z_0 be applied to the substrate. It is convenient to specify the structure of the coating in terms of the complex–valued function $\varepsilon\left(z,T\right)$, which described the permittivity distribution along the normal to the coating.

Any spatial orientation of the electrical and magnetic vectors with respect to the interface between the media can be reduced to the consideration of two basic versions: s- and p-polarization. For the fields inside an inhomogeneous coating, it is useful to normalize their amplitudes so that the electrical component of the transmitted wave has unit amplitude. Then the mathematical model can be formulated as the following Cauchy problem with initial condition at $z = 0$:

$$\frac{du}{dz} = i\kappa\upsilon \qquad \frac{d\upsilon}{dz} = i\kappa\left[\varepsilon\left(z,T\right) - \alpha^2\right]_u$$

$$u\big|_{z=0} = 1 \qquad \upsilon\big|_{z=0} = -p_0$$

in the case of s-polarization and

$$\frac{du}{dz} = i\kappa\left[1 - \frac{\alpha^2}{\varepsilon\left(z,T\right)}\right]\upsilon, \qquad \frac{d\upsilon}{dz} = i\kappa\varepsilon\left(z,T\right)u$$

$$u\big|_{z=0} = 1 \qquad \upsilon\big|_{z=0} = -p_0$$

for p-polarization. Here $\alpha = n_a \sin\theta$. (n_a is the refractive index of the external medium from which the wave reaches the surface), and the value of p_0 in initial condition depends on the polarization

$$p_0 = \begin{cases} \sqrt{{n_0}^2 - \alpha^2} & s-polarization \\ {n_0}^2\Big/\sqrt{{n_0}^2 - \alpha^2} & p-polarization \end{cases}$$

Since similar expressions will be used in the calculations below, we shall assume that for any j

$$p_j = \begin{cases} \sqrt{{n_j}^2 - \alpha^2} & s-polarization \\ {n_j}^2\Big/\sqrt{{n_j}^2 - \alpha^2} & p-polarization \end{cases}$$

In our problem, u corresponds to the amplitude of the electric field and υ to that of the magnetic field of the electromagnetic wave. Differential equations circumscribed above are direct consequences Maxwell's equations, transformed taking into account the spatial one-dimensional problem with a harmonic dependence of the fields on time of the form $\exp(-i\omega\tau)$. We will now write the expressions for the amplitude reflectance r and transmittance t

$$r = \left.\frac{p_a u + \upsilon}{p_a u - \upsilon}\right|_{z=z_0}, \qquad t = \left.\frac{z p_a}{p_a u - \upsilon}\right|_{z=z_0}$$

where the parameter p_a can be expressed in terms of the refractive index of the external medium n_a by formula

$$(p_a)_j = \begin{cases} \sqrt{{n_{aj}}^2 - \alpha^2} & s - polarization \\ {n_{aj}}^2 \Big/ \sqrt{{n_{aj}}^2 - \alpha^2} & p - polarization \end{cases}$$

The power reflectance and transmittance are equal to

$$R = |r|^2 \qquad t = \frac{R_e(p_0)}{R_e(p_a)}|t|^2$$

To formulate the synthesis problem, we introduce the objective functional Q, characterizing the rms distance between the spectral parameters obtained for the multiplayer system and the desired values:

$$\begin{aligned} Q(\varepsilon(z.T)) = \sum_{\{\kappa,\theta\}} \Big\{ & W_s^r(\kappa,\theta)\left[R_s(\kappa,\theta) - R_s(\kappa,\theta)\right]^2 + \\ & W_p^r(\kappa,\theta)\left[R_p(\kappa,\theta) - \tilde{R}(\kappa,\theta)\right]^2 + \\ & W_s^t(\kappa,\theta)\left[T_s(\kappa,\theta) - \tilde{T}_s(\kappa,\theta)\right]^2 + \\ & W_p^t(\kappa,\theta)\left[T_p(\kappa,\theta) - \tilde{T}_p(\kappa,\theta)\right]^2 \Big\} \end{aligned}$$

The summation is carried out over a prescribed finite set of values of wave numbers and angles of incidence $\{\kappa,\theta\}; R_s(\kappa,\theta), R_p(\kappa,\theta), T_s(\kappa,\theta), T_p(\kappa,\theta)$ are the power reflectances and transmittances of the coating for s- and p-polarization respectively, and $R_s(\kappa,\theta), R_p(\kappa,\theta), T_s(\kappa,\theta), T_p(\kappa,\theta)$ is the required form of those coefficients. In synthesis problems, expression for $Q(\varepsilon(z,T))$ for the objective functional is usually introduced as a quadrature formula, approximating the integral with respect to a continuous set of values of the wave numbers. In that expression, the coefficients of the quadrature formula are taken as weights $W\begin{Bmatrix} r,T \\ s,p \end{Bmatrix}$ but this can be varied by the user during synthesis to obtain the best solution for their purposes.

The problem of synthesizing a multiplayer system in very general form can be states as follows:

$$\varepsilon(z.T) = \arg\inf_{\varepsilon(z.T)\in\mathcal{E}} Q\left[\varepsilon(z.T)\right]$$

where $\mathcal{E}$ is a set subject to the physical and technological constraints imposed on the form of the function $\varepsilon(z.T)$. In practice, multiplayer systems most often have a piecewise-constant distribution $\varepsilon(z.T)$ as they consist of N inhomogeneous layers. If the permittivity of each layer is fixed, the system as a whole can be characterized uniquely by the vector of thickness $\mathrm{X} = \{d_j\}$. Thus the functional Q becomes a function of N variables and the synthesis problem can be reformulated in the form

$$\mathrm{X}_{opt} = \arg\inf_{\mathrm{X}\in p} Q[\mathrm{X}]$$

where the set P is defined by the physical constraints.

The calculations can be made more concise by considering the following general optimal control problem.

Suppose we have the Cauchy problem

$$\frac{dx}{dz} = f(x,\varepsilon) \qquad 0 < z < z_a$$

$$x\big|_{z=0} = x^{(0)}$$

The real valued objective functional is defined at the right-hand end $z = z_a$ on the solution of system above $Q = Q(x(z_a))$. The functional $Q(x(z_a))$ will take the form $Q(x(t_a))$ where *t* is a new independent variables.

The specific detail of the method will be explained below, but here we obtain general expressions for the first and second variations of the functional Q for small variations of the non-negative function $\rho(t)$. As a result of our calculation we can show that the first variation is defined by the linear term in δ on the right-hand side of transformed expression

$$\Delta Q = Q(\rho_b(t)) - Q(\rho(t))$$

as

$$\delta Q = -\delta\left[\operatorname{Re}\int_0^{t_a} \eta(t) H(\psi,x,\varepsilon) dt\right]$$

and the second variation can be written up to terms $O(\delta^2)$ in the form

$$\delta^2 Q = -\delta \operatorname{Re}\int_0^{t_a} \eta(t)\left\langle f_x^+\psi + \frac{1}{2}\theta f + \frac{1}{2}\xi f^*, \Delta x\right\rangle dt$$

where ψ is vector function.

III. NUMERICAL RESULTS

Second order optimization is an important feature of the programs for synthesizing multilayer coating for PC developed here. In addition the method of acicular variations, the basic idea of which was described in [1], has been used. To a considerable extent the acicular variations procedure is heuristic, and so the programs provide a flexible interface with the user, based on a menu system and the input of screen patterns.

The system is provided with a graphic monitor for the solution procedure, which greatly simplifies the analysis of the results and enables use to be made of the users intuitive knowledge during the actual solution of the applied problem.

An interactive, but not totally formulated method of constructing solutions for problems of synthesizing multiplayer coating is quite natural from the practical point of view. The point is that the very concept of an optimum solution of the synthesis problem is impossible to formulate copmletely. For a fixed number of layers, it is reasonable to interpret an optimum solution as one, which gives the global minimum of the estimator function. However, the number of layers is not usually known in advance. The larger the number of layers, naturally, the deeper the global minimum will be. But by contrast the number of layers should be as small as possible for practical implementation of the results. Since in most cases it is impossible to estimate the relation between the achievable accuracy of the approximation of the spectral dependences and the number of layers beforehand, the dimensions of the solution space cannot be fixed before synthesis starts. There is not space here to describe all the possibilities and heuristic methods used to construct quasi-optimal solutions.

We will now compare the efficiency of the CG method and MNM [6] using the algorithm for the rapid computation of the matrix of second derivatives described above. Computation of the matrix of second derivatives takes from 10 units for 20 variables to 12 units for 45 variables. We will conclude by giving some examples of the solution of one real applied problem:

1. To synthesize a non-reflective coating on a glass substrate (n_0=1.52) for λ=0.4-0.9mμ and $0^0 \le \theta < 30^0$. One result obtained is a coating of 16 layers of geometric thickness 9.95H, 47.70L, 28.00H, 21.35L, 109.67H, 15.60L, 27.46H, 65.23L, 10.43H, 103.98L, 22.12H, 31.76L, 78.44H, 15.69L, 30.45H, 109.62L the thickness of all the layers is given in nm, the letter H and L indicate the material from which the respective layers are made: H denotes TiO_2 with refractive indices $2.2 \le n \le 2.4$ and L denotes MgF_2 $(1.37 \le n \le 1.39)$. The graphics of power reflectances against frequency for angles of incidence between $0^0 \le \theta \le 30^0$ are shown in figure 1.

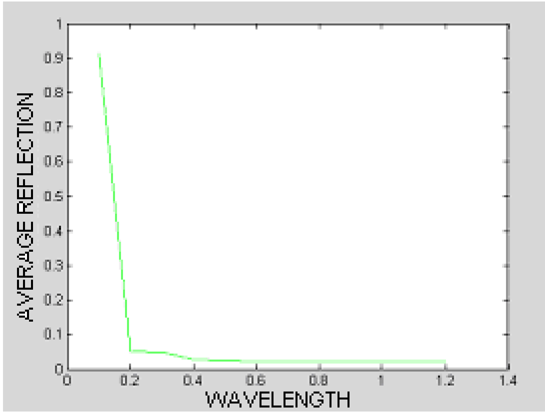

Figure 1. Spectral dependence of reflection from multilayers structure

IV. CONCLUSION

The result obtained for this problem by the widely known FCALC program (written by Goldstein) is a 24-layer coating. With our result, we obtained a series of 16 and 22-layers solutions which were comparable with the 24-layer coating in accuracy of approximation of the required spectral dependence.

V. REFERENCES

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