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Use of the theory of coupled waves for constructing multilayer optical coatings

P.A. Kholokhonova, P.E. Tverdokhleb

***Abstract*. A general numerical method is proposed for constructing multilayer optical coatings without using the basic structure. The possibility of application of the theory of coupled waves for describing optical coatings with a large difference in the values of the refractive index is demonstrated. As design parameters, the coefficients of harmonic expansion of the required functions $n(x)$ are used, which makes it possible to produce local variations in a certain spectral region. The method is quite pictorial. An example of application of this method for calculating a broadband divider is considered.**

Keywords: *multilayer optical coating, coupled-wave theory*.

1. Introduction

A multilayer optical coating is a system of dielectric layers with various thicknesses and refractive indices. The coordinate dependence $n(x)$ of the refractive index will be referred to as the structure of optical coating, while the dependence of the reflectance R (or transmittance T) on the wave number $k = 2\pi/\lambda$ will be referred to as its spectral characteristic.

The problem of constructing a multilayer optical coating involves the determination of the structure, which satisfies the required spectral characteristics and which can be implemented.

The existing methods for constructing thin-film coatings can be classified as universal and special [1 – 3]. Universal methods can be used for calculating any optical coating, while special methods are used to calculate coatings of a special type. The calculation technique (numerical or analytical) is also an important characteristic of the method.

At present, numerical computer techniques have become a powerful tool for designing, which often exceed the potentialities of analytic methods. The numerical method essentially involves the variation of design parameters to optimise a given target function. Such parameters are usually the thickness and the refractive index of each layer. We will refer to these quantities as microparameters because they determine the structure of an individual layer rather that the entire structure.

Numerical methods make it possible to obtain very accurate results as regards the extent to which spectral characteristics of the resultant structure approach the specified values. For this reason, the major part of these methods employs special numerical algorithms, in which individual features of the structure are used [4 – 7].

There also exist very powerful special analytic methods (for example, for calculating chirped mirrors [8]). Among universal analytical methods, Fourier synthesis is the most widely used [9]. This is an approximate method that can be used for obtaining a structure with a gradient refractive index profile. However, because of its approximate nature, Fourier synthesis is used in practice not directly, but as the basis for an iterative numerical algorithm [10, 12]. Another powerful universal numerical method is the needle-shaped synthesis [13, 14]. Finally, numerous universal numerical methods are used for optimising a certain basic structure [15 – 17]. In some cases, a structure whose spectral characteristics are very close to required values, but do not satisfy a certain criterion (minimal/maximal layer thickness, accuracy, or stability) is chosen as the basic structure. In other cases, a basic structure of an elementary form is used for determining the starting values of design parameters.

The available design methods make it possible to solve most of the existing problems. However, a sequence of a few methods is commonly used for calculating the structure of the required coating because each of these methods cannot separately provide the optimal solution in an arbitrary case. An approximate solution is obtained using a method that does not require the presence of the basic structure. Then one of the methods of numerical optimisation is used, in which the approximate structure is used as the basis. For this reason, the development of universal methods that can be used for obtaining basic structures for subsequent optimisation remains an actual problem.

Below, we present a universal numerical method for designing multilayer optical coatings. This approach differs from most numerical methods because it employs as design parameters the coefficients of harmonic expansion of the required function $n(x)$ rather than the thickness and refractive index of each layer. Such a choice of design parameters (which will be referred to as macroparameters) was made on the basis of the results of the coupled-wave theory (CWT). This imparted an important feature to this method, i.e., the possibility of local variations in a certain range of dependences $R(k)$ and $T(k)$. In this case, the

P.A. Kholokhonova, P.E. Tverdokhleb Institute of Automation and Electrometry, Siberian Branch, Russian Academy of Sciences, prosp. akad. Koptyuga 1, 630090 Novosibirsk, Russia;
e-mail: kholokhonova@iae.nsk.su, peter@iae.nsk.su

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number of parameters being optimised is reduced by an order of magnitude. In this method, a transition to structures with a discrete refractive index profile is performed at once.

The coupled wave theory is applicable in the approximation of slowly varying amplitudes, i.e., under the conditions when the variation in the radiation-wave amplitude is negligibly small at a scale comparable with the perturbation period. For this reason, this theory was used as a rule for studying structures with a small relative perturbation of the refractive index. However, the application of the CWT for calculating the phase characteristics of optical coatings – structures with a large difference in the values of the refractive index was demonstrated in [8]. We will show below that the CWT can also be used for describing the amplitude characteristics of optical coatings.

This approach has much in common with the methods in which the Fourier synthesis relations and frequency filtration are used [10 – 12]; however, unlike these methods, the CWT is simpler and descriptive because it does not employ inverse integral relations and is reduced to solving a number of direct problems.

2. Theory

Before designing an optical coating, it is necessary to find the relation between $R(k)$ and $n(x)$. This relation can be established by using the CWT [18]. Because the CWT equations were derived with the help of the parabolic approximation of the wave equation, the application of these equations was usually limited to the study of structures with a small relative perturbation of the refractive index (for example, holographic gratings). It was shown in [8], however, that the CWT can be employed for describing phase characteristics of optical coatings with a large difference in refractive indices ($n_{\max} = 2.45$, $n_{\min} = 1.5$). The aim of the authors of [8] was to obtain exact expressions for phase characteristics of the structure using the CWT, which necessitated the introduction of certain changes in the classical formulas for the coupling and mismatch coefficients. Here, we confine our analysis to qualitative agreement between $R(k)$ and $n(x)$, which is described by the CWT, because unlike the analytic method employed in [8], our approach is based on numerical optimisation.

Consider briefly the basic principles of the CWT. For a propagating light wave, an optical coating is a perturbation of the medium, i.e., the region in which the refractive index depends on the coordinate, resulting in the appearance of a reflected wave. According to the CWT, the existence of a harmonic component with frequency $k_{0/2}$ (Fourier component) in the spatial structure of $n(x)$ leads to the formation of a reflection peak at a frequency of k_0 in the optical spectrum $R(k)$. This occurs due to the appearance of the effective coupling between the forward and backward waves at this frequency.

Let us expand the function $n(x)$ in Fourier series (assuming that this function is periodically continued):

$$n(x) = \sum_m \left[a_m \sin\left(\frac{2\pi m}{D} x\right) + b_m \cos\left(\frac{2\pi m}{D} x\right) \right] = \sum_m \left[a_m \sin(k_m x) + b_m \cos(k_m x) \right],$$

where D is the total optical thickness of the coating; a_m and b_m are the Fourier expansion coefficients; m is the Fourier harmonic number; $k_m = 2\pi m/D$; and x is the optical thickness. We will refer to harmonic expansion functions $\sin(k_m x)$ and $\cos(k_m x)$ as the basis functions.

Let us verify the correspondence between the Fourier spectrum and the optical spectrum $n(x)$ of the structure, which is predicted by the CWT. Let us assume that the dependence $n(x)$ is described by a single Fourier harmonic; in this case, only one Fourier coefficient is nonzero. Consider the structure for which the maximal and minimal refractive indices are equal to 2 and 1.45, respectively. By using the characteristic matrix formalism, we calculate the spectral characteristic of this structure (Fig. 1).

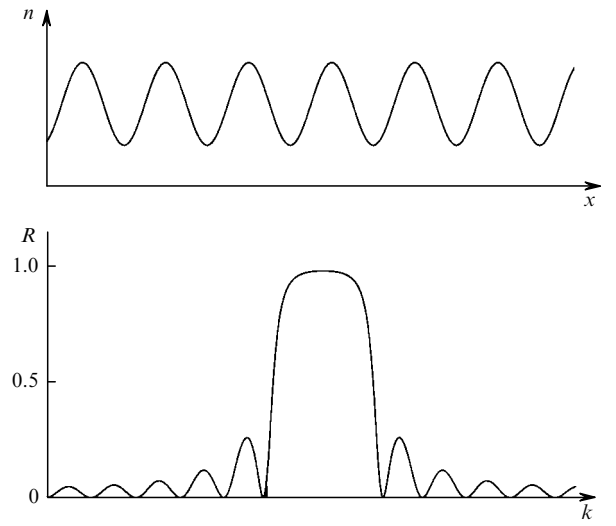

Figure 1. Coordinate dependence $n(x)$ of the refractive index described by a Fourier harmonic and the wavenumber dependence of the reflectance $R(k)$ (where $k = 2\pi/\lambda$).

The Fourier harmonic b_0 of the spatial spectrum of the structure corresponds to the reflection region in the optical spectrum $R(k)$. One can see that a qualitative agreement between $R(k)$ and $n(x)$ is also observed for an optical coating with a large difference between refractive indices. Thus, the application of harmonic expansion coefficients as macroparameters of the structure establishes a linear relation between $R(k)$ and $n(x)$. To form reflection regions at definite frequencies, it is necessary to 'construct' $n(x)$ from harmonic functions of the corresponding frequency.

Note that this approach substantially differs from most of numerical simulation methods. The structure is numerically selected by varying a microscopic parameter – the thickness of a single layer, which changes the optical spectrum in the entire frequency range. However, in our case, variation of a macroscopic parameter – the harmonic expansion coefficient results in changes of the entire profile $n(x)$, but this leads to variations within a certain spectral region. In other words, we can introduce 'local' variations.

The next step is the improvement of the obtained model algorithm and extension of its possibilities. To avoid the analysis of a smooth profile of the refractive index (which is of no practical importance), we approximate in our simulation the harmonic components (sinusoidal and cosinusoidal) by functions with a rectangular profile, which will be henceforth referred to as q functions.

Let us assume that the total thickness D of the structure and the maximum wavelength λ_0 of the range we are interested in are specified. Then the basis function of length D and period $\lambda_0/2$ will be called the zero-order basis function and denoted by $q_0(x)$. This function corresponds to the reflection peak at wavelength λ_0. All the remaining basis functions can be obtained from $q_0(x)$ using a similarity transformation (compression): $q_m(x) = q_0(\varkappa_m x)$, where $\varkappa_m = \lambda_0/\lambda_m$. Each of these functions corresponds to a reflectione peak at a wavelength of λ_m in the optical spectrum.

The basis functions have the same number of periods, but different carrier frequencies and total lengths D_m because these functions essentially represent the same parent function q_0 compressed with the corresponding coefficient. Figure 2 shows the functions $q_0(x)$ and $q_m = q_0(0.8x)$.

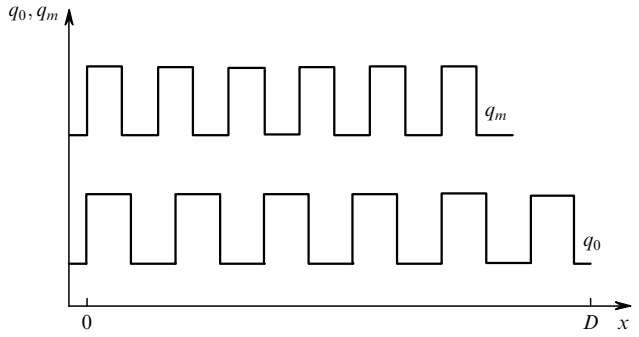

Figure 2. Basis functions $q(x)$ used for specifying the optical coating structure $n(x)$; $q_0(x)$ is the zero-order basis function, $q_m = q_0(0.8x)$ is an arbitrary-order basis function.

Because the parent function can be compressed with an arbitrary coefficient, the basis under study is continuous. Note, however, that the harmonic functions used here are not infinitely long, but are bounded by length D. These functions do not form a complete basis and, strictly speaking, are not independent; however, their interaction is not critical for designing and can be neglected.

Thus, the refractive index profile will be specified by a set of basis functions. Let us assume that the profile $n(x)$ is specified only by basis functions with coefficients b_m, i.e.,

$$n(x) = \sum_m b_m q_0(\varkappa_m x) = \sum_m b_m q_m(x).$$

The introduction of additional harmonics into the spatial spectrum of the structure ('Fourier' spectrum) gives rise to the corresponding reflection peaks in the optical spectrum. In simulation of such an optical coating, layers with refractive indices that do not correspond to real materials appear. For this reason, the obtained structure was transformed with the help of the Herpin algorithm [19] into a structure consisting of layers with two refractive indices. Figure 3 shows a structure specified by two q harmonics and the optical spectrum of this structure. Note that the peak value of the reflectance depends on the relative amplitude b_m of the corresponding q component and can be easily controlled.

As mentioned above so far, only structures with even basis functions were considered. The possibility of introducing basis functions with coefficients a_m (odd functions)

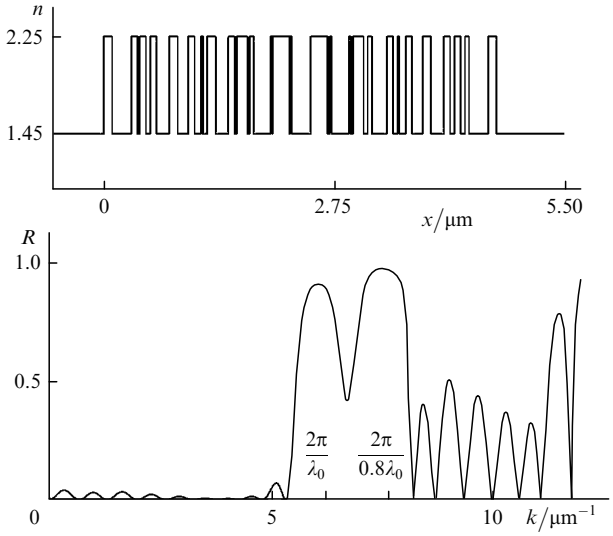

Figure 3. Structure of the optical coating $n(x)$ containing two q harmonics and the corresponding dependence $R(k)$ ($\lambda_0 = 1$ μm).

makes it possible to introduce one mode design parameter. The basis functions have the same number of periods, but different carrier frequencies and different total lengths D_m. Because $D_m < D$, we have an additional parameter in our disposal (referred to as the 'phase' parameter), namely, the displacement of basis functions relative to one another. By varying this parameter, we can control the interaction between the spectral components $q_m(x)$, namely, by combination or separation of the reflection peaks corresponding to them. Figure 4 shows the dependence $n(x)$ specified by two q functions with the relative displacement $0.143\lambda_0/2$ and the spectral characteristic $R(k)$ corresponding to it.

If, however, we change the shift of harmonic components relative to one another for the same values of the remaining parameters, we can obtain a single reflection region in the optical spectrum (Fig. 5). One can see from Fig. 5 that the reflection region has side peaks. This complicates the simulation procedure because the presence of oscillations near the reflection peak does not allow one to construct transmission regions in adjacent frequency ranges when it is required. The problem of elimination of undesirable side oscillations is well-known and can be solved using finite functions [20]. The solution of this problem is based on the wavelet analysis, according to which a set of finite functions (unlike infinite harmonics) is used for expansion. As the basis functions with a rectangular profile, the basis wavelet functions can be obtained from the parent function $V(x)$ by a the similarity (compressions) transformation: $\upsilon_m(x) = V(\varkappa_m x)$. In our case, we used functions of the form $\upsilon_m(x) = q_0(\varkappa_m x)\sin(\pi x/D)$. Let us express $n(x)$ in terms of functions $\upsilon_m(x)$, treating them as the basis functions:

$$n(x) = \sum_m b_m \upsilon_m(x).$$

Figure 6 shows the refractive index profile and the optical spectrum $R(k)$ for a structure containing a wavelet component of the form $\upsilon_0(x) = q_0(x)\sin(\pi x/D)$. One can see that the reflection peak in this case has no side peaks, which makes it possible to construct transmission regions along with high-reflection regions.

The drawback of the wavelet approach compared to the

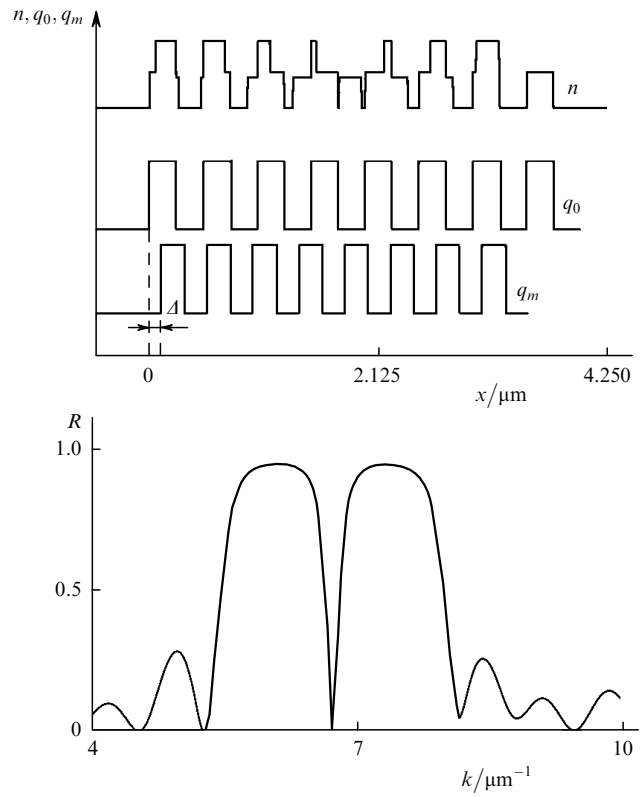

Figure 4. Structure of the optical coating $n(x)$ specified by two basis functions q_0 and q_m displaced relative to each other by $\Delta = 0.143\lambda_0/2$ and the corresponding dependence $R(k)$ ($\lambda_0 = 1$ μm).

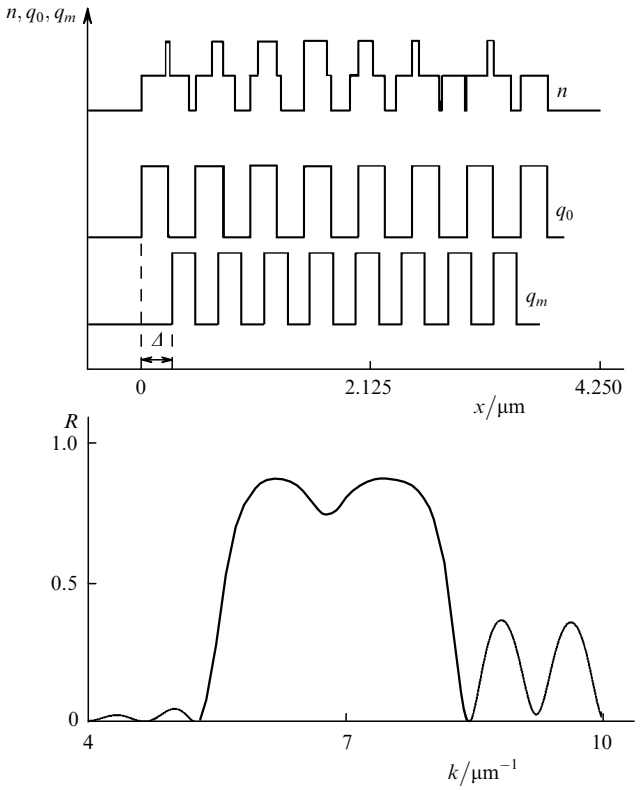

Figure 5. Structure of the optical coating $n(x)$ specified by two basis functions q_0 and q_m displaced relative to each other by $\Delta = 0.356\lambda_0/2$ and the corresponding dependence $R(k)$ ($\lambda_0 = 1$ μm).

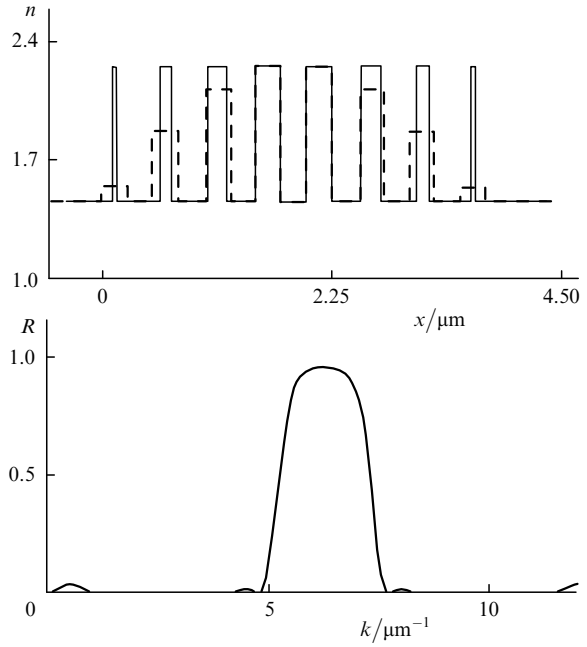

Figure 6. Structure of the optical coating $n(x)$ specified by a wavelet component υ_0 (calculated values of the refractive index; dashed curve) and the structure transformed with the help of the Herpin algorithm (solid curve) and the corresponding dependence $R(k)$.

application of q functions is the relatively small amplitude of reflection peaks for the same number of coating layers. Therefore, the wavelet representation is superfluous if the specified spectral characteristic does not contain regions in which high transmission would be important.

Thus, the method for constructing an optical coating with the specified spectral characteristic $R(k)$ by using macroparameters involves the following stages.

(i) Depending on the form of the specified function $R(k)$, the type of basis functions is chosen for the harmonic representation of $n(x)$. If the function $R(k)$ contains critical transmission regions, the wavelet expansion should be used. Otherwise, conventional rectangular functions are employed.

(ii) The number of layers described by the component functions $q_m(x)$ or $\upsilon_m(x)$, which provides the required values of $R(k)$ and/or $\mathrm{d}R(k)/\mathrm{d}k$ (steepness of the slopes) is determined.

(iii) The primary structure of $n(x)$ is formed by specifying amplitudes b_m of several basis functions, $q_m(x)$ or $\upsilon_m(x)$, whose frequencies are chosen proceeding from the arrangement of the reflection regions in the required $R(k)$ spectrum. Then the parameters are optimised by changing the amplitudes of the harmonics and their relative phases by introducing additional harmonics when required.

3. Application of the method

Let us illustrate the possibilities of our approach. Let us assume that a broadband optical divider has to be designed for operation in a wavelength range between 680 and 900 nm with a reflectance $R(\lambda) = 0.5 \pm 0.01$. The refractive indices of the layers are $n_\mathrm{L} = 1.45$, $n_\mathrm{H} = 2.25$. The refractive index of a substrate is $n_\mathrm{s} = 1.45$; the ambient medium is air ($n_\mathrm{a} = 1$). The difference between the refractive indices at the external coating – air interface is described by the expression

$$n(x) = \begin{cases} n_s, & x \leqslant 0, \\ n_a, & x > 0. \end{cases}$$

The spectral characteristic of the optical divider designed in this way and shown in Fig. 7 satisfies the requirements formulated above. The working range is 250 nm, which makes it possible to use such a divider in femtosecond laser systems. The difference in the reflectances in the working range is less than 1 %.

The method considered here can be also used for calculating other thin-film optical elements like comb filters or broadband reflecting coatings.

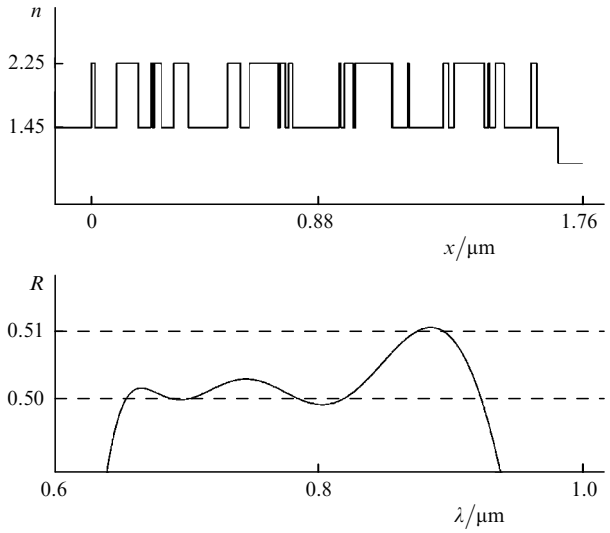

Figure 7. Structure $n(x)$ of an optical divider and the corresponding dependence $R(\lambda)$.

4. Conclusions

We have proposed a universal numerical method for constructing multilayer optical coatings. The possibility of application of the CWT for describing optical coatings with a large difference in the refractive indices in the case when the slowly varying amplitude approximation is violated is demonstrated. A specific feature of this method is the possibility of using the harmonic expansion coefficients of the required function $n(x)$ as design parameters, which makes it possible to produce local changes in a certain spectral region and to reduce substantially the number of parameters being optimised. The method is simple and descriptive. The possibilities of the method have been illustrated by the example of designing a broadband optical divider.

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