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Computationally Efficient Algorithm for Designing Multilayer Dielectric Gratings

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Abstract—A new computationally efficient algorithm for designing multilayer dielectric gratings (MDG) is developed based on the previously proposed modified method of separation of variables for solving direct problem of diffraction of electromagnetic waves by MDG structures. The performance of the proposed algorithm is demonstrated by designing an MDG element for spectral beam combining applications. The considered MDG element is based on on a pair of practically promising thin film materials.

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1. INTRODUCTION

Multilayer dielectric gratings (MDG) are among the most technologically advanced elements of modern optical and optoelectronic applications [1–5]. In high power laser applications, MDG elements have almost completely replaced traditional metal gratings due to their much better resistance to high intensity laser radiation [6]. Basically, MDG elements are combinations of one-dimensional multilayer dielectric structures with 2- or 3-dimensional gratings formed in the upper dielectric layer. Designing of such elements is a computationally demanding problem, since it requires multiple solutions of the direct problem of diffraction of an electromagnetic wave by MDG elements.

Until now, the rigorous coupled-wave analysis [5–8] and the finite-difference method [9] have been widely used to solve the direct diffraction problem. In [10], to increase the computational efficiency of solving the direct problem, a new modified method of separation of variables was proposed. Its accuracy has been confirmed by the comparison with the results obtained using the traditional rigorous coupled-wave analysis. In this paper, we report a computationally efficient algorithm based on this method and applied to design a special type of multilayer dielectric gratings, namely MDG elements for spectral beam combining.

Spectral beam combining (SBC) is a promising technique for achieving extremely high laser power. It uses MDG elements to combine multiple incoherent laser beams, usually diode laser beams of different

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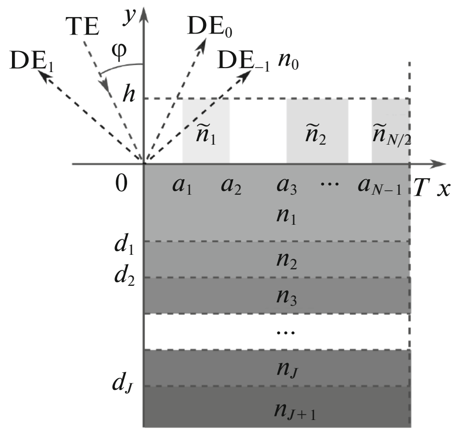

Fig. 1. Schematic representation of MDG.

wavelengths, into one intense beam. In [5], excellent prospects for the use of MDG elements based on a pair of materials Si : H and SiO_2 for SBC applications were demonstrated. In this paper, we consider such MDG elements to demonstrate the effectiveness of the proposed algorithm.

The paper is organized as follows. Section 2 presents the formulation of the direct problem and describes the main steps of the proposed algorithm. Section 3 provides the results demonstrating the performance of the algorithms for SBC applications. The final Section 4 presents the main conclusions.

2. MATHEMATICAL ALGORITHM

Consider the MDG schematically depicted in Fig. 1. An electromagnetic wave with TE polarization is incident on the MDG element consisting of a periodic rectangular grating and a sequence of multilayer dielectric films. The parameters of the considered element change only in the Oxy plane.

The grating period is $T > 0$, the grating height is $h > 0$. There are $N/2$ lines in each grating period. The lines have different widths. In general, their refractive indices can also be different.

A TE-polarized wave is obliquely incident on the MDG structure at an incidence angle φ. The electric field can be represented using only the longitudinal component of the field. Let $u_0(x, y)$ denote this component of the incident wave. The incident electric field can be written as

$$u_0(x, y) = \exp\left(-ik_0 n_0 \left(x \sin\varphi - (y - h)\cos\varphi\right)\right),$$

where $k_0 = 2\pi/\lambda_0$ and n_0 are the wave-number and the refractive index of free space, λ_0 is a wavelength. Let us introduce a refractive index $n(x, y)$ equal to n_0 everywhere outside the MDG for $y \in (0, h)$ and to $\tilde{n}_i$ in the grating lines, where $i = \overline{1, N/2}$. Here $N > 0$ is an even integer. For $y < 0$, $n(x, y)$ is equal to n_j in the layers of the multilayer structure ($j = \overline{1, J}$, and $J \geqslant 0$ is the number of layers).

The direct problem of diffraction is to find the longitudinal component of the total electric field $u(x, y)$ that satisfies the Helmholtz equation

$$\left(\Delta + k_0^2 n^2(x, y)\right) u(x, y) = 0,$$

continuity conditions at the grating surfaces and at the boundaries of layers, radiation conditions at infinity, Floquet condition

$$u(x, y) = \exp\left(ik_0 n_0 T \sin\varphi\right) u\left(x + T, y\right),$$

and the condition of finiteness of energy in each bounded spatial domain. It is also required to determine the diffraction efficiency of the main diffraction orders [7, 11].

Using the plane wave method [7], we represent the nonzero component of the electric field in the form

$$u^{(0)}(x, y) = u_0(x, y) + \sum_{l=-\infty}^{+\infty} r_l z_l(x) \exp\left(-ik_{0,yl}(y - h)\right), \ y > h, \tag{1}$$

$$u^{(j)}(x,y)=\sum_{l=-\infty}^{+\infty} z_l(x)\left(p_l^{(j)}\exp\left(ik_{j,yl}(y-d_j)\right)+q_l^{(j)}\exp\left(-ik_{j,yl}(y-d_j)\right)\right),\ y\in(d_j,d_{j-1}),\quad (2)$$

$$u^{(J+1)}(x,y)=\sum_{l=-\infty}^{+\infty} t_l z_l(x)\exp\left(ik_{J+1,yl}y\right),\ y<d_J,\quad (3)$$

where $z_l(x):=\exp(-ik_{xl}x)$, $j=\overline{1,J}$, $d_0=0$,

$$k_{j,yl}=\begin{cases}\sqrt{k_0^2n_j^2-k_{xl}^2}, & k_0n_j\geqslant|k_{xl}|,\\ -i\sqrt{k_{xl}^2-k_0^2n_j^2}, & k_0n_j<|k_{xl}|,\end{cases}\qquad j=\overline{0,J+1},$$

and the k_{xl} values are determined using the Floquet condition and are given by the expressions $k_{xl}=k_0n_0\sin\varphi-\frac{2\pi l}{T}$, l is integer. It follows from (3) that $p_l^{(J+1)}\equiv t_l$, $q_l^{(J+1)}\equiv 0$.

It can be proved that all coefficients $p_l^{(j)}$ and $q_l^{(j)}$ can be represented using t_l, where t_l is the unknown normalized electric-field amplitude of the forward-diffracted (transmitted) wave in the region $y<d_{J+1}$ and r_l is the unknown normalized electric-field amplitude of the l-th backward-diffracted (reflected) wave in the region $y>h$.

In rectangles $\Pi_j=(a_j,a_{j+1})\times(0,h)$, where $j=\overline{0,N-1}$ and $a_0=0$, $a_N=T$, the values of the wavenumber are different: $\kappa_{2j}=k_0n_0$, $\kappa_{2j+1}=k_0\tilde{n}_{j+1}$, $j=\overline{0,N/2-1}$, (see Fig. 1). The width of the grating lines $\Delta_j=a_{j+1}-a_j$ ($j=\overline{0,N-1}$) is not constant, i.e. irregular gratings are considered.

Let us formulate the mathematical algorithm for solving the problem based on modified method of separation of variables [10].

Let M be positive even value. First of all we numerically obtain approximate eigenvalues $\lambda=\lambda_l$, $l=\overline{-M/2,M/2}$ by solving equation

$$\det(I-QS_{N-1}\dots S_0)=0,\quad (4)$$

where

$$S_j=\begin{pmatrix}\frac{\gamma_j(\lambda)}{\gamma_{j+1}(\lambda)}\cos(\gamma_j(\lambda)\Delta_j) & -\frac{\gamma_j(\lambda)}{\gamma_{j+1}(\lambda)}\sin(\gamma_j(\lambda)\Delta_j)\\ \sin(\gamma_j(\lambda)\Delta_j) & \cos(\gamma_j(\lambda)\Delta_j)\end{pmatrix},\quad j=\overline{0,N-1},$$

$$Q=\exp\left(ik_0n_0T\sin\varphi\right)\begin{pmatrix}\frac{\gamma_{N-1}(\lambda)}{\gamma_0(\lambda)}\cos(\gamma_{N-1}(\lambda)\Delta_{N-1}) & -\frac{\gamma_{N-1}(\lambda)}{\gamma_0(\lambda)}\sin(\gamma_{N-1}(\lambda)\Delta_{N-1})\\ \sin(\gamma_{N-1}(\lambda)\Delta_{N-1}) & \cos(\gamma_{N-1}(\lambda)\Delta_{N-1})\end{pmatrix},$$

I is an identity matrix of size 2,

$$\gamma_j(\lambda)=\begin{cases}\sqrt{\kappa_j^2-\lambda}, & \kappa_j^2\geqslant\lambda,\\ i\sqrt{\lambda-\kappa_j^2}, & \kappa_j^2<\lambda,\end{cases}\qquad j=\overline{0,N-1}.$$

The left-hand side of equation (4) is a complex-valued function. At the same time the solutions of equation (4) $\lambda=\lambda_l$, $l=\overline{-M/2,M/2}$ are real values. Therefore equation (4) can be represented as system

$$\begin{cases}\Re\big(\det(I-QS_{N-1}\dots S_0)\big)=0,\\ \Im\big(\det(I-QS_{N-1}\dots S_0)\big)=0.\end{cases}\quad (5)$$

A modified shooting method is used to determine the solutions of system (5), based on the search for a simultaneous sign reversal of left-hand sides of the equations of system (5).

Further, we can determine constants $c_{j,l}$, $d_{j,l}$, $j=\overline{0,N-1}$, $l=\overline{-M/2,M/2}$ by formula

$$(c_{j+1,l},d_{j+1,l})^T=S(c_{i,l},d_{i,l})^T,\quad j=\overline{0,N-2},$$

where $(c_{0,l}, d_{0,l})^T$ is any nontrivial solution of system

$$(c_{0,l}, d_{0,l})^T = QS_{N-1}\dots S_0(c_{0,l}, d_{0,l})^T$$

for $\lambda = \lambda_l$. On the next step, we have two equations for $b_l^{(1)}$, $b_l^{(2)}$ $(l = \overline{-M/2, M/2})$

$$\sum_{p=0}^{M} X_{p,l}\big(ik_{0,yl}Y_p(h) + Y_p'(h)\big) = iT\big(k_{0,yl} + \cos\varphi\big), \tag{6}$$

$$\sum_{p=0}^{M} X_{p,l}\Big(ik_{1,yl}\big(\tilde{p}_l - \tilde{q}_l\big)Y_p(0) - \big(\tilde{p}_l + \tilde{q}_l\big)Y_p'(0)\Big) = 0, \tag{7}$$

where

$$X_{p,l} = \sum_{s=0}^{N-1} z_l(a_s)T\Big(T^2\gamma_s^2(\lambda_l) - (2\pi l - T\sin\varphi)^2\Big)^{-1}\Big(c_{s,l}\gamma_s(\lambda_l)T + d_{s,l}i\big(2\pi l - T\sin\varphi\big)$$
$$- c_{s,l}z_l(\Delta_s)\Big(i\big(2\pi l - T\sin\varphi\big)\sin(\gamma_s(\lambda_l)\Delta_s) + T\gamma_s(\lambda_l)\cos(\gamma_s(\lambda_l)\Delta_s)\Big)$$
$$- d_{s,l}z_l(\Delta_s)\Big(i\big(2\pi l - T\sin\varphi\big)\cos(\gamma_s(\lambda_l)\Delta_s) - T\gamma_s(\lambda_l)\sin(\gamma_s(\lambda_l)\Delta_s)\Big)\Big),$$

the function Y_l has the form

$$Y_l(y) = b_l^{(1)}\exp\big(iy\sqrt{\lambda_l}\big) + b_l^{(2)}\exp\big(-i(y-h)\sqrt{\lambda_l}\big).$$

Constants $\tilde{p}_l = \tilde{p}_l^{(1)}\exp\big(-ik_{1,yl}d_1\big)$, $\tilde{q}_l = \tilde{q}_l^{(1)}\exp\big(ik_{1,yl}d_1\big)$, where, taking into account (2), (3), $\tilde{p}_l^{(1)}$, $\tilde{q}_l^{(1)}$ are determined by relations

$$\tilde{p}_l^{(j)} = \frac{1}{2}\left(\tilde{p}_l^{(j+1)}P_l^{(j+1)} + \tilde{q}_l^{(j+1)}Q_l^{(j+1)} - \frac{k_{j+1,yl}}{k_{j,yl}}\left(\tilde{p}_l^{(j+1)}P_l^{(j+1)} - \tilde{q}_l^{(j+1)}Q_l^{(j+1)}\right)\right),$$
$$\tilde{q}_l^{(j)} = \frac{1}{2}\left(\tilde{p}_l^{(j+1)}P_l^{(j+1)} + \tilde{q}_l^{(j+1)}Q_l^{(j+1)} + \frac{k_{j+1,yl}}{k_{j,yl}}\left(\tilde{p}_l^{(j+1)}P_l^{(j+1)} - \tilde{q}_l^{(j+1)}Q_l^{(j+1)}\right)\right)$$

at $\tilde{p}_l^{(J+1)} \equiv 1$, $\tilde{q}_l^{(J+1)} \equiv 0$, where $P_l^{(j)} := \exp\left(ik_{j,yl}(d_{j-1} - d_j)\right)$, $Q_l^{(j)} := \exp\left(-ik_{j,yl}(d_{j-1} - d_j)\right)$, $j = \overline{1, J}$, $P_l^{(J+1)} := \exp\left(ik_{j,yl}d_J\right)$, $Q_l^{(J+1)} := \exp\left(-ik_{j,yl}d_J\right)$.

System (6), (7) can be represented in the matrix form

$$W\mathfrak{b} = \mathfrak{f}, \tag{8}$$

where $\mathfrak{b} = (b_{-M/2}^{(1)}, \dots, b_{M/2}^{(1)}, b_{-M/2}^{(2)}, \dots, b_{M/2}^{(2)})^\top$ and the coefficients of the matrix $W = \big(w_{i,j}\big)_{(2M+2)\times(2M+2)}$ and the vector $\mathfrak{f} = (f_1, f_2, \dots, f_{2M+2})^\top$ are determined from the system (6), (7) in the following form

$$w_{j,p} = i\exp\big(ih\sqrt{\lambda_l}\big)X_{p,l}\big(k_{0,yl} + \sqrt{\lambda_l}\big),$$
$$w_{j,M+1+p} = iX_{p,l}\big(k_{0,yl} - \sqrt{\lambda_l}\big),$$
$$w_{M+1+j,p} = iX_{p,l}\Big(k_{1,yl}\big(\tilde{p}_l - \tilde{q}_l\big) - \big(\tilde{p}_l + \tilde{q}_l\big)\sqrt{\lambda_l}\Big),$$
$$w_{M+1+j,M+1+p} = i\exp\big(ih\sqrt{\lambda_l}\big)X_{p,l}\Big(k_{1,yl}\big(\tilde{p}_l - \tilde{q}_l\big) + \big(\tilde{p}_l + \tilde{q}_l\big)\sqrt{\lambda_l}\Big),$$

where $l = -M/2 + j$, $j, p = \overline{0, M}$,

$$f_j = 0, \quad j = 1, 2, ..., M/2, M/2+2, ..., 2M+2, \quad f_{M/2+1} = iT\big(k_{0,yl} + \cos\varphi\big).$$

To solve the system of $2M+2$ linear equations (8), the Gauss–Jordan method is used.

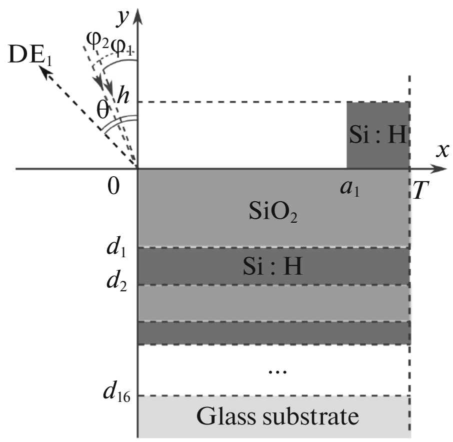

Fig. 2. Schematic of a multilayer dielectric grating for spectral beam combining in the spectral range of 1000–1100 nm. The diffraction angle for the first diffraction order is 45 degrees, the range of incidence angles for the selected wavelength range is from 23.82 to 31 degrees. The grating period T is 900 nm.

Using (1)–(3), we can calculate the amplitudes t_l and r_l by equations

$$t_l = T^{-1}\big(\tilde{p}_l - \tilde{q}_l\big)^{-1} \sum_{p=0}^{M} X_{p,l} Y_p(0), \quad l = \overline{-M/2, M/2},$$

$$r_l = T^{-1} \sum_{p=0}^{M} X_{p,l} Y_p(h), \quad l = -M/2, ..., -1, 1, ..., M/2,$$

$$r_0 = T^{-1} \sum_{p=0}^{M} X_{p,0} Y_p(h) - 1.$$

Finally we obtain the diffraction efficiency in the lst diffraction order determined by formula

$$DE_l = |r_l|^2 \Re\Big(\frac{k_{0,yl}}{k_0 n_0 \cos\varphi}\Big) + |t_l|^2 \Re\Big(\frac{k_{J+1,yl}}{k_0 n_0 \cos\varphi}\Big).$$

3. RESULTS AND DISCUSSION

The proposed algorithm is implemented as a c++ code using parallel computations. The eigenvalues $\lambda = \lambda_l$, $l = \overline{-M/2, M/2}$ are determined in parallel on several threads. The number of threads depends on the characteristics of the processor. For 10 threads and $M = 6$, the program runtime is 0.2 seconds.

The efficiency of the proposed algorithm was tested by designing an MDG element for spectral beam combining in a wide spectral band from 1000 to 1100 nm. In our calculations, we used a pair of Si : H/SiO_2 thin film materials. Silica dioxide (SiO_2) is a widely used thin film material with low refractive index. At the same time, the hydrogen-dopped silicon (Si : H) has not yet been systematically used in thin film optics as a material with high refractive index. Its use was made possible by a technological process, briefly described below. As shown later in this section, the main advantage of using a selected pair of materials is the very high contrast in their refractive indices.

The Si : H/SiO_2 multilayer films can be effectively fabricated using an ion-beam sputtering deposition system [5]. In the process, silicon is the starting material, H_2 and O_2 are injected during the deposition to reduce structural defects and voids in thin films of amorphous Si that cause absorption at low photon energies. This makes it possible to use Si : H with low absorption in the near-infrared region.

Based on the experimental results obtained at Tongji University, we use the following refractive indices for the selected pair of materials: $n = 1.48$ for SiO_2 and $n = 3.52$ for Si : H.

A general configuration of the designed MDG element is shown in Fig. 2. The direction angle θ for the first diffraction order is chosen equal to 45 degrees. Based on this value, the range of incidence angles

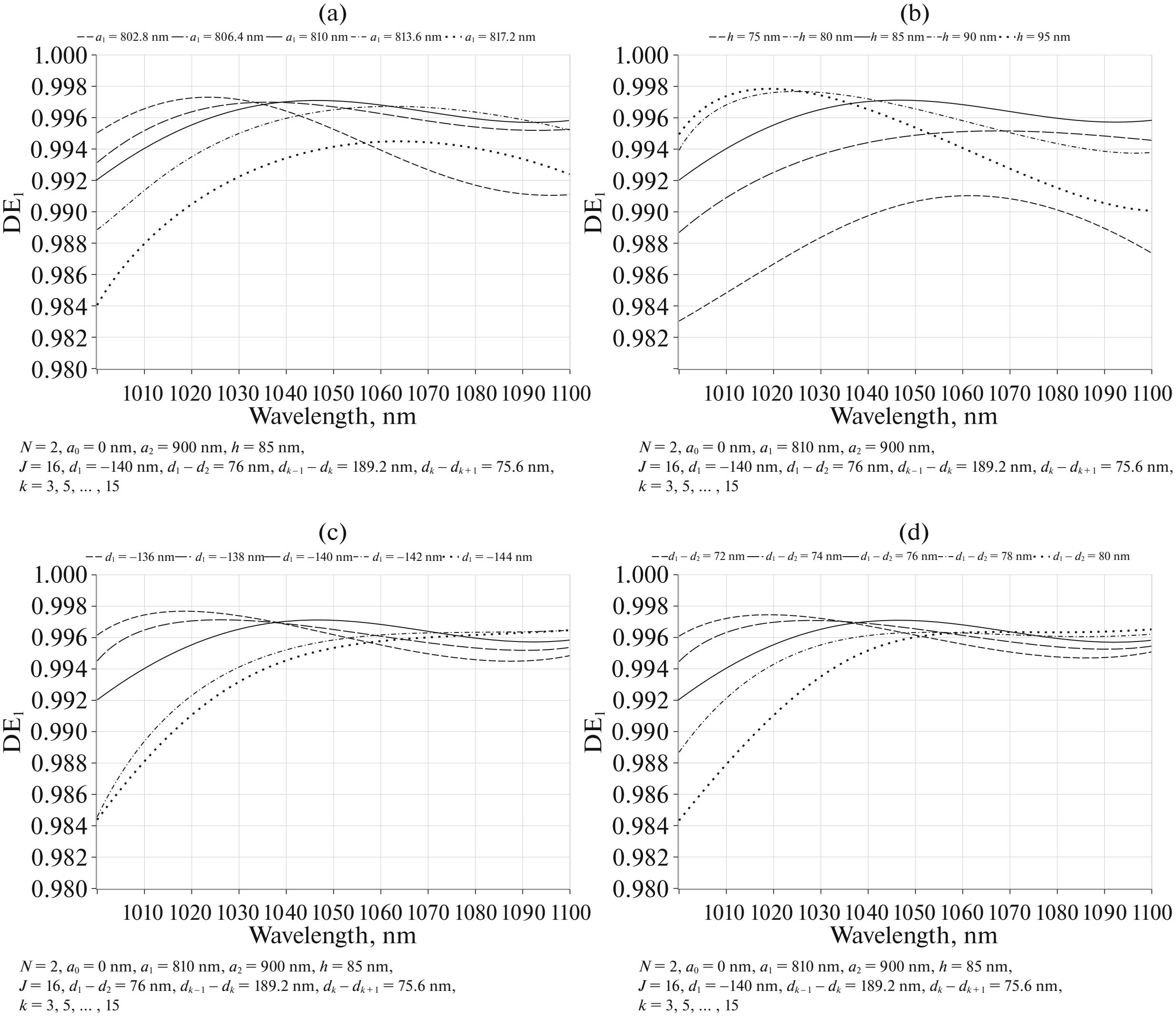

Fig. 3. Dependencies of the diffraction efficiency in the first diffraction order on the main design parameters: (a) width of the grating groove a_1, (b) height of the grating line h, (c) thickness of the first matching layer (SiO_2 layer), (d) thickness of the second matching layer (Si : H layer). Parameters of the quarter wave mirror are indicated in the text. The substrate refractive index is 1.458.

for the selected wavelength range is from 23.82 to 31 degrees. The grating period T is set to 900 nm, which ensures that for the selected wavelength range there is only one propagating diffracted wave in the first diffraction order.

The main purpose of using multilayer dielectric mirrors in MDG elements is to prevent energy diffraction in the substrate on which the MDG element is formed. In our case, this is a grey medium at the bottom of Fig. 2. The high refractive index contrast of a pair of Si : H/SiO_2 thin film materials provides a high reflectance and a high width of the reflection zone of a quarter wave dielectric mirror based on this pair of materials. The quarter wave mirror is formed by fourteen layers deposited on the substrate with alternating refractive indices of 3.52 and 1.48. The thicknesses of its layers are chosen so as to provide the maximum width of the high reflection zone at an incidence angle of 30 degrees (this is the average value for the considered range of incidence angles—see Fig. 2). They are 75.6 nm for the Si : H layers and 189.2 nm for the SiO_2 layers. There are two more thin layers at the top of the quarter wave mirror. These two layers are often refereed to as «matching layers» and their main purpose is to destroy the resonance effects that can occur in the layers between the quarter wave mirror and the diffraction grating. This is achieved by varying the thicknesses of these upper layers, which are therefore important design parameters of the MDG element.

Another advantage of using Si : H as a high index material is that the diffraction grating formed in the upper Si : H layer can have much smaller depth than in the case of commonly used high refractive index materials [5]. The height of the grating line h and the width of the grating groove a_1 are two other design parameters of the MDG element under consideration.

The excellent computational performance of the developed algorithm allows a detailed study of the dependencies of the diffraction efficiency in the first diffraction order on the main design parameters of the MDG element. The results of this study are shown in Fig. 3.

From Figs. 3a and 3b, it can be seen that both the height of the grating line and the width of the grating groove are important design parameters and that the diffraction efficiency is very sensitive to their changes. The thicknesses of the matching layers (see Figs. 3c and 3d) are also important, but their variations lead to similar effects, which should be expected, since these variations mainly affect the phases of the waves reflected by the underlying dielectric mirror. Thus it is possible that for some applications only one matching layer can be used (this reduces the number of design parameters).

In general, the diffraction efficiency in the considered wide spectral range exceeds 99.4%. For the most important laser wavelengths, it may be even higher. An MDG element with $h = 85$ nm, $a_1 = 810$ nm, and thicknesses of the first and second matching layers of 140 nm and 76 nm, respectively, provides a diffraction efficiency in the first diffraction order equal to 99.69% for the wavelength of 1054 nm and 99.63% for the wavelength of 1064 nm.

4. CONCLUSION

A computationally efficient algorithm for solving the direct problem of the diffraction of electromagnetic waves by MDG structures has been developed. The algorithm is based on the previously proposed modified method of separation of variables. A feature of the proposed mathematical algorithm is that numerical procedures are used only to calculate the auxiliary problem of finding eigenvalues, and the main stages of the algorithm are implemented analytically. This yields that we minimize approximate calculations in the process of solving the problem and obtain a numerical-analytical algorithm. The developed algorithm is well suited for parallelization. It is implemented as c++ code using parallel computations.

The computational efficiency of the developed algorithm was tested by designing an MDG element for spectral beam combining of laser beams in a wide spectral range from 1000 to 1100 nm. A practically promising pair of Si : H/SiO_2 thin film materials was used in calculations. A high level of diffraction efficiency has been achieved in the considered spectral range, as well as at the most important laser wavelengths.

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