Development of a software package for modeling and analysis of light diffraction on periodic structures of nanophotonics by the rigorous coupled-wave analysis

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Abstract. We discuss the development of a software package, which enables simulating and analyzing the diffraction of a plane electromagnetic wave on a multilayer diffraction grating with. The main functional requirements to the system are formulated. The architectural solution of the implemented software including the main functional and logical layers of the system with the specified methods of their interaction is described. The method allowing one to model light diffraction on multilayer diffraction structures comprising homogeneous layers and diffraction gratings with one-dimensional periodicity is implemented. A polarizing reflector consisting of a diffraction grating on a Bragg grating (a one-dimensional photonic crystal) consisting of a small number of layers is designed and investigated. The optimal parameters of the structure are found for a given reflectance criterion. The parameter ranges satisfying the chosen criterion are investigated. The influence of changes in the geometric parameters of the structure on the reflector performance is discussed. The designed software package is promising for the design of grating-based nanophotonic filters and sensors.

1. Introduction

During the last decade, photonics has been one of the most rapidly developing areas of modern physics. Due to the complexity of the theoretical description and experimental studies of nanophotonic structures, the development of methods and software tools for rigorous numerical simulation of the diffraction of electromagnetic radiation on such structures is particularly important.

At present, diffraction gratings are widely used as cornerstone elements of various optoelectronic systems and devices, in particular, spectral and spatial filters and laser resonators. In these devices, multilayer structures containing diffraction gratings and homogeneous layers are utilized. The configurations of such structures are determined on the basis of the required qualitative and quantitative characteristics by rigorously modeling diffraction of light on these structures. The purpose of this work is to design and implement a software package that enables simulating and investigating the diffraction of a plane electromagnetic wave on a multilayer diffraction grating, the configuration of which is determined by the user. As an application example of the developed software, we discuss the design of a polarization-selective mirror comprising a diffraction grating and a one-dimensional photonic crystal.
2. Software implementation

2.1. Functional requirements to the developed software system

Any simulation of a physical process requires the specification of the input data, the calculations, and the analysis of the obtained data: it is necessary to set the parameters and configuration of the simulated structure, to simulate mathematically the investigated physical process(es), to estimate the accuracy of the computational method, and to analyze the simulation results.

In this work, the simulated process is the diffraction of a plane electromagnetic wave on a multilayer grating. The modeling involves several main stages, consideration of which will allow one to formulate the main functional requirements to the software being developed.

Let us list the main functional requirements to the application:

1) The interface should allow the user to define the characteristics of the incident electromagnetic wave (polarization, wavelength and angle of incidence with respect to the normal to the layer interfaces). The superstrate and substrate media, in which the diffraction grating is located, are described by the refractive indices. The multilayer grating is described by the layer thicknesses, refractive indices and fill factors.

2) The user interface should enable the tracking of the progress of the performed calculations. For this, a tracking service based on websockets [1] has to be implemented, since it will allow the application client to monitor the progress of calculations in the “real-time” mode.

3) The user interface should implement features for analyzing the performed calculations. For example, the interface should allow drawing graphs of the energy characteristics (diffraction order intensities) of the simulated diffraction of the electromagnetic radiation on the configured grating. The graphs should be implemented using Plotly.js [2], due to its high configurability. The interface must operate with data obtained through the REST API [3] provided by the server.

2.2. Software system architecture

On the basis of the formulated requirements to the software package being implemented, it is necessary to define its program structure as a set of functional modules. The system being developed should divide the mentioned functions between the individual modules for the ease of use, testing and support. Therefore, the architectural structure of the developed software consists of the components presented in figure 1.

![Figure 1. Software architecture of the developed modeling system.](image)
The interface capabilities are implemented in the web layer of the application. This application uses the Angular Framework [4], which enables the development of an application within a component model, in which the application corresponds to a hierarchy of interrelated components.

The “business layer” of the system being developed is a Java server application. The web part of this application is organized using the Spring Framework, which provides all the features of a web application with component-based functional separation between its parts based on the concept of dependency injection. The REST API is implemented by the REST controllers of the application, which associate an HTTP request of a specific format with a class method of the controller. The controller can call the methods of the application components through the CDI mechanism [5]. Using this mechanism, the controller accesses services that are responsible for the different functions. In this application, the main services are the service for obtaining the previously calculated simulation results and the service for running calculations with progress tracking.

It is important to note that the data server itself does not simulate the wave diffraction: this function is assumed by the computational core. This is a separate computing server that provides an API for calculating the energy characteristics (diffraction order intensities) of a grating of a given configuration in a known environment. All the necessary calculations are carried out using an own implementation of the Fourier modal method, which is briefly described below, in the Python 3.5 programming language. For the mathematical calculations, the library NumPy is utilized.

This modular structure has the following advantages:
1) client-server interaction: the data processing is separated from the client layer;
2) modularity: the individual functions of the application are divided into separate structural parts, which ensures their high interchangeability;
3) testability of the independent modules of the system;
4) extensibility: when developing other computational processes related to the developed one, it is easier and safer to implement new functionalities required from the system;
5) low binding and high connectivity: REST API, which regulates the interaction of the application levels, clearly divides the functional responsibilities between them.

3. Method for numerical simulation of diffractive structures containing homogeneous layers and one-dimensional diffraction gratings

There is a large number of works dedicated to the rigorous numerical solution of the diffraction problem on periodic structures [6–12]. In this work, the Fourier modal method (FMM, also known as rigorous coupled-wave analysis, RCWA) is used in combination with a stable algorithm for simulating the diffraction of an electromagnetic wave by a set of plane-parallel layers. Let us briefly describe the method for the case of TE-polarization.

We consider the case when a TE-polarized electromagnetic wave with a unit amplitude and a free-space wavelength \( \lambda_0 \) is obliquely incident at an angle \( \alpha \) on a multilayer diffraction grating. The grating is bound by two different media with refractive indices \( n_I \) and \( n_H \). In this case, the electric field component of the incident wave that is normal to plane of incidence is given by

\[
E_y = \exp \left[ -jk_0 n_I (x \sin \alpha + z \cos \alpha) \right].
\]

where \( k_0 = 2\pi/\lambda_0 \). The corresponding components of the reflected and transmitted electric fields are given by

\[
\begin{align*}
E_{n+} &= E_y + \sum_i R_i \exp \left[ -j (k_{\omega i} x - k_{\omega i} z) \right], \\
E_{n-} &= \sum_i T_i \exp \left[ -j (k_{\omega i} x - k_{\omega i} (z - d)) \right],
\end{align*}
\]

where \( k_{\omega i} \) is determined from the Floquet condition [13] and is given by

\[
k_{\omega i} = k_0 \left( n_I \sin \alpha - i \frac{2\pi}{\Lambda} \right),
\]

where \( \Lambda \) is the grating period.
In Eq. (2), \( R_i \) and \( T_i \) are the normalized amplitudes of the \( i \)-th transmitted and reflected diffracted orders in the corresponding media.

Note that the magnetic field in each region may be obtained from the Maxwell-Faraday equation

\[
\vec{H} = \frac{j}{\omega \mu} \mathbf{rot} \vec{E},
\]

where \( \mu \) is the absolute magnetic permeability of the medium.

Let us consider the field in the grating. In the grating layer with the index \( l = 1, L \), where \( L \) is the number of grating layers, the amplitudes of the tangential components may be expressed as the following Fourier expansions:

\[
E_{i,i}(x) = \sum_{n \geq 1} S_{i,i,n}(z) \exp \left( -jk_{l,i}x \right),
\]

\[
H_{i,i}(x) = -j \sqrt{\mu_0} \sum_{n \geq 1} U_{i,i,n}(z) \exp \left( -jk_{l,i}x \right).
\]

By substituting these expansions into the Maxwell’s equations, we obtain the set of differential equations for a particular layer

\[
\frac{\partial \delta^2 S_{i,l}}{\partial z^2} = A S_{i,l},
\]

where \( z = k_qz \), \( A \), \( K = K^2 - \mathbf{E} \), \( \mathbf{K} \) is the diagonal matrix of the values \( k_{l,i}/k_0 \), and \( \mathbf{E} \) is the Toeplitz matrix formed by the Fourier coefficients of the dielectric permittivity \( \varepsilon_i \).

We solve the set of equations (8) by calculating the eigenvalues and eigenvectors associated with the matrix \( A \). The space harmonics of the tangential electric and magnetic fields in the grating region are then given by

\[
S_{i,n}(z) = \sum_{n \geq 1} w_{i,j,n} \left[ c^+_{i,n} \exp \left( -k_{l,i}q_{l,n} (z - D_i + d_i) \right) + c^-_{i,n} \exp \left( k_{l,i}q_{l,n} (z - D_i) \right) \right],
\]

\[
U_{i,n}(z) = \sum_{n \geq 1} v_{i,j,n} \left[ -c^+_{i,n} \exp \left( -k_{l,i}q_{l,n} (z - D_i + d_i) \right) + c^-_{i,n} \exp \left( k_{l,i}q_{l,n} (z - D_i) \right) \right],
\]

where \( w_{i,j,n} \) are the elements of the eigenvector matrix \( \mathbf{W}_i \), \( q_{l,n} \) are the elements of the singular values matrix \( \mathbf{Q}_i \), \( v_{i,j,n} \) are the elements of the matrix \( \mathbf{V}_i = \mathbf{W}_i \mathbf{Q}_i \); \( c^+_{i,n} \) and \( c^-_{i,n} \) are the unknown constants to be determined from the boundary conditions; \( d_i \) is the layer thickness, and \( D_i \) is the total layer thickness up to and including the considered \( l \)-th layer.

Writing the boundary conditions in the matrix form, we obtain a system of linear equations for calculating the desired amplitudes of the reflected and transmitted diffracted waves:

\[
\begin{pmatrix}
\delta_{n,0}
\end{pmatrix} = \begin{pmatrix}
I
\end{pmatrix} \mathbf{R} \begin{pmatrix}
\delta_{n,0}
\end{pmatrix} + \begin{pmatrix}
-I
\end{pmatrix} \mathbf{T},
\]

where \( \delta_{n,0} \) is the Kronecker delta, and \( \mathbf{x}_i, \mathbf{z}_i, \mathbf{z}_u \) are the diagonal matrices with the elements

\[
\exp \left( -k_{l,i}q_{l,n}d_i \right), \quad k_{l,i}/k_0 \quad \text{and} \quad k_{l,i}/k_0, \quad \text{respectively.}
\]

Note that each multiplier of the product on the right side of Eq. (11) contains one inversion of the matrix, which can be ill-conditioned at a large value of
To avoid this problem, we decompose the analytically invertible matrix, consider the last factor of it and make a substitution:

$$\begin{bmatrix} a_l \\ b_l \end{bmatrix} = \begin{bmatrix} W_L & W_L \end{bmatrix}^{-1} \begin{bmatrix} f_{l+1} \\ g_{l+1} \end{bmatrix}; T = a_L^{-1} X_L T_L. \tag{12}$$

where $f_{l+1} = I$, $g_{l+1} = jZ_L$. With this substitution, the last factor in Eq. (11) is reduced to

$$\begin{bmatrix} f_L \\ g_L \end{bmatrix} T = \begin{bmatrix} W_L (I + X_L a_L^{-1} X_L) \\ V_L (I - X_L b_L a_L^{-1} X_L) \end{bmatrix} T_L. \tag{13}$$

Repeating the process for the remaining layers of the diffraction grating, Eq. (11) is transformed to

$$\begin{bmatrix} \delta_{\alpha} \\ n_j \cos \alpha \delta_{\alpha} \end{bmatrix} + \begin{bmatrix} 1 \\ -jZ_L \end{bmatrix} R = \begin{bmatrix} f_L \\ g_L \end{bmatrix} T_L, \tag{14}$$

and then $T = a_L^{-1} X_L \times \ldots \times a_0^{-1} X_T.$

The equations (14) are solved without numerical instabilities for any number of grating layers with arbitrary thicknesses.

To determine the intensities of the diffraction orders, we find the ratio of the absolute values of the z-components of the time-averaged Poynting vector to the corresponding value of the incident wave. In the case of TE-polarization, such components are given by

$$S = \frac{E_x H_z^*}{2}. \tag{15}$$

For the incident wave, this component has the form

$$S_{inc} = \frac{k_a n_a \cos \alpha}{2 \omega \mu_a}. \tag{16}$$

For the reflected and transmitted diffraction orders, these components are given by

$$S_{R,T} = \frac{\text{Re} k_{\xi \psi} \int R \text{Re} k_{\xi \psi}}{2 \omega \mu_a}, S_{T,R} = \frac{\text{Re} k_{\mu \psi} \int T \text{Re} k_{\mu \psi}}{2 \omega \mu_a}. \tag{17}$$

Thus, the intensities of the diffraction orders are defined as

$$DE_k = \frac{k_a n_a \cos \alpha}{k_a n_a \cos \alpha}, DE_T = \frac{\text{Re} k_{\xi \psi} \int R \text{Re} k_{\xi \psi}}{k_a n_a \cos \alpha}, \tag{18}$$

The sum of the intensities of the diffraction orders must be unity for lossless gratings and does not depend on the number of space harmonics retained in field expansion.

Thus, the described method enables calculating the intensities of diffraction orders for analyzing the performance of the diffraction structure being simulated.

4. Investigation of a polarizing reflector based on a diffraction grating and a photonic crystal

4.1. Problem statement

In a number of tasks of optoelectronic technology and laser optics (for example, in laser ranging) polarization-selective mirrors (PSMs) are used. These reflectors provide the required levels of reflectance of each of the polarizations (TE and TM) at the working wavelength. One of the used configurations is based on a diffraction grating on the surface of a one-dimensional photonic crystal. This is due to the fact that a photonic crystal with properly chosen parameters works as a Bragg mirror and effectively reflects the required range of wavelengths, whereas the diffraction grating allows the reflector to “react” to the polarization of the incident radiation.
The geometry of the considered PSM is presented in figure 2. It is a diffraction grating deposited on a system of plane-parallel homogeneous layers. The simulated PSM has the following parameters: the Bragg grating consists of alternating MgF₂ layers (refractive index 1.38) and TiO₂ (refractive index 2.47) with quarter-wave thicknesses on a quartz (refractive index 1.48) substrate. A binary TiO₂/air diffraction grating is deposited on this multilayer structure. On this structure, a plane wave with either TE- or TM-polarization with a wavelength of 1064 nm is normally incident.

The task is to find such parameters of the structure (the number of Bragg grating periods, the diffraction grating period and height), at which the reflectance of a TE-polarized wave would be as close to 100% as possible (over 99%), and the reflectance of a TM-polarized wave would not exceed 80%. Note that this criterion does not limit the lower reflectance threshold of the TM polarization. Let us also mention that the used reflectance criterion was taken from a real design problem concerning the application in laser ranging.

4.2. PSM parameters calculation
Using the FMM, let us simulate the diffraction of a normally incident wave on the structure under consideration. To analyze the fulfillment of the given criterion for the reflectance of the TE- and TM-polarizations, let us calculate the dependence of reflectance on the wavelength normalized by the period of the diffraction grating and on its height also normalized by the period. Let us calculate the following dependencies: the intensity of the zero reflected diffraction order for each of the polarizations and their difference (top three graphs in figure 3) and carry out the threshold processing of these dependencies in accordance with the specified reflectance criterion, and the selection of points satisfying the criterion (bottom three graphs in figure 3). Let us increase the number of layers of the Bragg grating in order to form a wide region of acceptable PSM parameters satisfying the criterion. An increase in the number of periods of the multilayer structure leads to the formation of a region of acceptable parameters, at which the reflectance values satisfy the criterion. In figure 3, which corresponds to seven periods of the Bragg grating, there are regions, where the difference in reflectance for the two polarizations reaches 99.7%.

As the “optimal” parameters of the PSM, we will choose the following values from one of the regions satisfying the criterion: the grating period is 1031 nm and the grating height is 634 nm.

To explain the obtained results, let us calculate the intensities of the zeroth and first transmitted diffraction orders. The calculated dependencies are presented in figure 4. It is evident that the low reflectance of the TM-polarization is due to the fact that the main part of the energy of the incident TM-polarized wave is directed to the ±1-st transmitted diffraction orders.
Figure 3. Reflectance (zeroth diffraction order) vs. normalized wavelength and grating height of the structure containing a diffraction grating and a seven-period Bragg grating for TE-polarization (a), TM-polarization (b), their difference (c) and images obtained using the threshold processing of the corresponding distributions according to the used criterion (d), (e), (f).

Figure 4. Intensities of the zeroth reflected diffraction order for TE- and TM-polarizations (a), (d), zeroth transmitted diffraction order for TE- and TM- polarizations (b), (e) and first transmitted diffraction order for TE- and TM- polarizations (c), (f).

Note that the reason for this effect is the existence of a photonic band gap in a multilayer structure under the grating, in which the modes of the photonic crystal are evanescent and do not propagate [14, 15]. This zone for the TE-polarization can be found from the dispersion relation of the photonic crystal:
\[
\cos(kd) = \cos(k_{1z}h_1)\cos(k_{2z}h_2) - \frac{k_{1z}^2 + k_{2z}^2}{2k_{1z}k_{2z}}\sin(k_{1z}h_1)\sin(k_{2z}h_2),
\]

where \(h_1\) and \(h_2\) are the thicknesses of the layers, \(d\) is the total thickness of the two layers (the period of the Bragg grating), and \(k_{1z} = (2\pi/\lambda)\sqrt{\eta_z^0 - \eta_{1z}^2}\).

The condition \(\cos(kd) > 1\) defines the photonic bandgap. Note that in the case of the TM-polarization, the dispersion relation has the same form, but \(k_{1z}\) in the rational function in the right part is replaced by \(k_{2z}/\eta_{1z}^0\). Let us calculate the dependencies of the right-hand side of the dispersion relations for different polarizations on the effective refractive index. The calculated dependencies are shown in figure 6. The vertical line in the graph indicates the effective refractive index equal to 1.033 and corresponding to the ±1-st diffraction orders. The region above the horizontal line defines the photonic bandgap; according to the points of the intersection of the effective refractive index line with the curves for the two polarizations, it can be seen that in the case of the TM-polarization, the first diffraction orders are not in the bandgap, whereas in the case of the TE-polarization they are. This explains the high intensity of the transmitted first orders in the case of the TM-polarization in figure 6.

Also note that the region of the “first-order diffraction” in the forbidden zone of the TE-polarization with the allowed first order of the TM-polarization is wide enough with respect to the effective refractive index (from 0.81 to 1.17), which determines the width of the acceptable region from figure 5.

According to figure 4, the “optimal” values of the PSM parameters are the following values: the grating period is 1031 nm and the grating height is 634 nm. These values correspond to the difference of 99.7% between the reflectance of TE- and TM-polarizations, which satisfies (and even exceeds) the chosen criterion.

Let us study the effect of changing the geometric parameters of the structure on its optical properties. Note that the central wavelength of 1064 nm is the local minimum of the reflectance of the TM-polarization, and the structure has a fairly wide wavelength range, in which the reflectance of the TM-polarization does not exceed 20% (from 1040 to 1110 nm).

In addition, there is even a wider range of values of the period of the diffraction grating, at which the reflectance of the TM polarization does not exceed 30% (from 877 to 1055 nm), which does not impose significant restrictions on the period of the diffraction grating to be fabricated. Similarly, the selected “optimal” value of the grating height of 634 nm is a local minimum, and around this value,
there is a wide range of values, at which the reflection of the TM-polarization does not exceed 20% (from 500 to 700 nm), which is also beneficial for the fabrication process.

In addition to these characteristics, one can vary the fill factor of the diffraction grating. In the simulations, it was assumed that the grating is binary with an equal width of the grating ridges and the grooves between the ridges. However, the simulations show that, firstly, it is possible to vary the fill factor (the ratio of the ridge width to the period) from 0.24 to 0.59, having a reflectance of the TM-polarization of 20%, and, secondly, there is another local minimum (0.25), where the reflection is less than 0.5%.

5. Conclusion
In this work, the main functional requirements to the software system for rigorous numerical simulation of the diffraction of plane electromagnetic waves on multilayer diffractive structures were formulated, and the architectural solution of the implemented software system was described. The Fourier modal method for simulating diffraction on multilayer structures containing homogeneous layers and diffraction gratings with one-dimensional periodicity was described and implemented. A polarizing reflector consisting of a diffraction grating on the surface of the Bragg grating consisting of a small number of periods was simulated and investigated. For a chosen reflectance criterion of TE- and TM-polarizations, the acceptable range of the parameters satisfying the criterion was investigated. The effect of changing the geometric parameters of the structure on the performance of the reflector is discussed. The simulations demonstrate that the considered polarizing reflector can meet a quite strict criterion concerning the reflectance levels and has large tolerances with respect to the geometrical parameters.

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