

LASER APPLICATIONS AND OTHER TOPICS IN QUANTUM ELECTRONICS

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Fast numerical method for modelling one-dimensional diffraction gratings

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Abstract. **Based on the generalised source method, a new method for calculating the light diffraction on one-dimensional dielectric diffraction gratings with an arbitrary profile is proposed. The method is an alternative to the widely used Fourier modal method because it possesses the same possibilities in defining different grating profiles; however, it has a significant advantage in calculating complex-shaped gratings because it requires many fewer mathematical operations. The applicability of the method is shown by comparing the calculation results by this method with the results obtained by the conventional methods of light diffraction calculation on the gratings.**

Keywords: *generalised source method, diffraction, diffraction gratings, Fourier modal method.*

1. Introduction

The possibility of exact diffraction simulation of periodic structures with different profiles is an extremely important task for many applied problems of modern optics [1]. In addition, the calculation methods of diffraction gratings has been recently used to study nonperiodic structures – separate elements of diffraction and integral optics [2–5]. The use of artificial periodicity in such problems seems justified because it allows one to evaluate the searched-for solutions in those regions where the conventional calculation methods of electromagnetic characteristics of separate nonperiodic elements having the dimensions comparable with the incident radiation wavelength are inapplicable.

Among numerical methods of different diffraction gratings, the most popular today are the Fourier modal method (FMM) [6, 7], its American variant – rigorous coupled wave approach (RCWA) [8], and the finite-difference time-domain or frequency-domain methods [1]. The FMM has a number of unique features making it possible to specify different grating profiles, is simple in realisation and well adequate for studying structures with the characteristic periods much smaller than the wavelength of radiation incident on them as well as comparable with this wavelength or slightly exceeding it. This method allows one to search for eigenmodes (diffraction orders) of the diffraction grating in the space of its inverse vectors. The main disadvantage of the method (inherent in all modal methods [9]) consists in the fact that its computational complexity (the number of operations needed to realise the algorithm) depends on the number N of the diffraction orders as N^3. This means that the increase in the number of grating periods required for considering the nonperiodic structures, and hence the increase in the number of diffraction orders lead to the fact that the applicability limits of the method are rapidly achieved even when powerful computers are used. Nevertheless, this method often proves to be more preferable than finite-difference schemes, which hardly take into account the physical character of specific problems and require huge memory capacities to analyse complex-shaped gratings.

Apart from the above approaches to diffraction grating calculations, note also the modal method [9, 10], Chandezon [9, 11] and Rayleigh [12] methods. The modal method, unlike the FMM, is used to search for the genuine grating modes but has the same disadvantage: the computational complexity increases with increasing the number of modes. In addition, the necessity of constructing the modal basis limits its applicability, in fact, to gratings with a rectangular profile. Application of this method is justified, for example, when it is needed to calculate the local fields with a high accuracy and to study the accuracy of some general method by the example of rectangular gratings. The Chandezon and Rayleigh methods are based on the possibility of representing the field in the grating region with the help of plane waves. These methods make it possible to calculate accurately another specific problem, i.e., gratings whose profiles are represented by smooth functions. In this connection, the Chandezon and Rayleigh methods are often used to analyse sinusoidal gratings.

Therefore, to study the optical properties of complex-shaped nonperiodic elements of diffraction and integral optics by the periodic-structure calculation methods, it is necessary to overcome the above-mentioned computational complexity limit N^3. In this paper we propose an approach to calculation of light diffraction on the gratings, which is an alternative to the conventional FMM and allows one to decrease significantly the computational complexity of the problem – down to $N \log N$. The new method is based on the generalised source method (GSM) [13] and reduces the problem to a self-consistent system of linear algebraic equations. This system of equations is solved with the help of the generalised minimal residual (GMRES) method [14], and the peculiar features of the matrices obtained by the GSM make it possible to perform matrix-vector multiplications in GMRES with the help of the fast Fourier transform (FFT) [15]. To model diffraction of 2D objects, the authors of paper [16] proposed a similar fast algorithm in which the Fredholm integral equation of convolution type is solved iteratively or with the help of the FFT.

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2. Analytic solution

Advantage is taken of the generalised source method [13] to derive analytic expressions which are used to construct the numerical solution of the problem. The method represents a scheme intended for solving the problems of electromagnetic radiation propagation in inhomogeneous media. It can be described as a sequence of two steps. Consider the function $\varepsilon(\boldsymbol{r})$ describing a spatially inhomogeneous permittivity which corresponds to the problem under study. First, the problem to be studied is replaced by another one whose geometry and permittivity distribution do not strongly differ from initial ones but which has an exact solution of Maxwell's equations for any current distribution $\boldsymbol{J}(\boldsymbol{r})$:

$$\boldsymbol{E}_{\mathrm{b}} = \aleph_{\mathrm{b}}(\boldsymbol{J}), \tag{1}$$

where $\aleph_{\mathrm{b}}$ is some linear operator. This solution will be called below basic and the function $\varepsilon_{\mathrm{b}}(\boldsymbol{r})$ corresponding to it will be called the basic permittivity distribution.

The second step of the generalised source method is used to search for the desired solution for the problem with $\varepsilon(\boldsymbol{r})$ in the form

$$\boldsymbol{E} = \boldsymbol{E}_0 + \aleph_{\mathrm{b}}(\boldsymbol{J}_{\mathrm{gen}}). \tag{2}$$

Here, $\boldsymbol{E}_0$ is the radiation field incident on the radiating system, and the generalised source is

$$\boldsymbol{J}_{\mathrm{gen}} = -\mathrm{i}\omega\Delta\varepsilon\boldsymbol{E}, \tag{3}$$

where $\Delta\varepsilon = \varepsilon - \varepsilon_{\mathrm{b}}$. Thus, relation (2) becomes an implicit self-consistent equation for unknown fields $\boldsymbol{E}$:

$$\boldsymbol{E} = \boldsymbol{E}_0 + \aleph_{\mathrm{b}}(-\mathrm{i}\omega\Delta\varepsilon\boldsymbol{E}). \tag{4}$$

In paper [17] the generalised source method was used to construct the numerical method for calculating light scattering from separate dielectric nanoparticles. In this paper, this method is used to calculate diffraction on one-dimensional plane gratings with the known profile.

First, in accordance with the GSM logics, we should choose the basic medium, the basic solution, and to obtain the explicit form of equation (2). To do this, we will consider a plane one-dimensional grating of depth h with a period Λ, located in the xy plane and periodic along the x axis. Assume first of all that the grating under study is located in a homogeneous isotropic medium with the permittivity ε_{b}, which will be used as basic one (changes induced by the presence of two different media from both sides of the grating are discussed below). Then, the solution of Helmholtz equation for the vector potential $\boldsymbol{A}$ under assumption that the Lorentz gauge is used, has the form of a convolution [18]:

$$\boldsymbol{A} = \mu_0\boldsymbol{J} * G = \int_{V'}\mu_0\boldsymbol{J}(\boldsymbol{r}')G(\boldsymbol{r}-\boldsymbol{r}')\mathrm{d}V', \tag{5}$$

where integration is performed over the region of the current existence;

$$G(\boldsymbol{r}) = \frac{\exp(\mathrm{i}k_{\mathrm{b}}|\boldsymbol{r}|)}{4\pi|\boldsymbol{r}|} \tag{6}$$

is the Green function of the scalar Helmholtz equation [18]; $k_{\mathrm{b}} = \omega\sqrt{\varepsilon_{\mathrm{b}}\mu_0}$. Hereafter, the factor $\exp(-\mathrm{i}\omega t)$ is omitted to save room.

To obtain the explicit form of (2) with the help of (5), we should take into account that the current in the one-dimensional periodic structure can be expanded in a sum of spatial harmonics:

$$\boldsymbol{J}(x,y,z) = \sum_{n=-\infty}^{\infty}\boldsymbol{j}_n(z)\exp(\mathrm{i}k_{xn}x + \mathrm{i}k_{y0}y), \tag{7}$$

where $k_{xn} = k_{x0} + nK = k_{x0} + 2\pi n/\Lambda$; k_{x0} and k_{y0} are the wave vector components of an incident wave exciting the current (7). Substituting (7) into (5) and expressing the electric field components by the potential, we derive the desired relation for spatial harmonics of the electric field components:

$$E_{\alpha n}(k_{xn},z) = \frac{\delta_{\alpha z}}{\mathrm{i}\omega\varepsilon_{\mathrm{b}}}j_{zn}(z)$$
$$+\omega\varepsilon_{\mathrm{b}}\sum_{\beta=x,y,z}\Big\{Y^{+}_{\alpha\beta n}\int_{-\infty}^{z}j_{\beta n}(z')\exp[\mathrm{i}k_{zn}(z-z')]\mathrm{d}z'$$
$$+Y^{-}_{\alpha\beta n}\int_{z}^{\infty}j_{\beta n}(z')\exp[-\mathrm{i}k_{zn}(z-z')]\mathrm{d}z'\Big\}. \tag{8}$$

Here, $\alpha, \beta = x, y, z$; $k_{zn} = \sqrt{k_{\mathrm{b}}^2 - k_{xn}^2 - k_{y0}^2}$; $Y^{\pm}_{\alpha\beta n} = (k^{\pm}_{\alpha n}k^{\pm}_{\beta n} - k_{\mathrm{b}}^2\delta_{\alpha\beta})/2k_{zn}$. The wave vectors $\boldsymbol{k}^{\pm}_n = \langle k_{xn}\ k_{y0} \pm k_{zn}\rangle^{\mathrm{T}}$ correspond to the waves in the positive and negative directions along the z axis. Note that apart from the plane harmonics in the entire space, field (8) of source (7) contains the correction in the source region and physically corresponds to the discontinuity of the normal field component in the planes perpendicular to the z axis.

For convenience of further considerations, we will introduce the modified field which, unlike (8), is expressed everywhere by the superposition of the plane waves:

$$\tilde{E}_{x,yn}(k_{xn},k_{y0},z) = E_{x,yn}(k_{xn},k_{y0},z),$$
$$\tilde{E}_{zn}(k_{xn},k_{y0},z) = E_{zn}(k_{xn},k_{y0},z) - \frac{j_{zn}(z)}{\mathrm{i}\omega\varepsilon_{\mathrm{b}}}. \tag{9}$$

In this case, in accordance with (3)

$$\tilde{E}_z = E_z + \frac{\Delta\varepsilon E_z}{\varepsilon_{\mathrm{b}}} = \frac{\varepsilon}{\varepsilon_{\mathrm{b}}}E_z, \tag{10}$$

i.e., the z-component of the modified field coincides with the electric induction with an accuracy to a constant, and hence is continuous on any plane parallel to xy.

Since the plane waves in the structures under study are the basic solutions in terms of the GSM, it is convenient to start considering TE- and TM-polarised harmonics instead of the electric and magnetic field components. Let us introduce the amplitude vectors of TE waves $a_n^{\mathrm{e}\pm}$ and TM waves $a_n^{\mathrm{h}\pm}$

$$\boldsymbol{a}_n^{\pm} = \langle a_n^{\mathrm{e}\pm}\ a_n^{\mathrm{h}\pm}\rangle^{\mathrm{T}}, \tag{11}$$

where the sign '±' shows the direction of their propagation along the z axis. Then, denoting the amplitude vectors of plane harmonics of the incident by $\boldsymbol{a}^{\pm}_{\mathrm{inc}}(z)$ and taking into account (9) and (11), we will rewrite expression (8) in the form:

$$\boldsymbol{a}_n^{\pm}(z) = \delta_{n0}\boldsymbol{a}^{\pm}_{\mathrm{inc}}(z) + \int_{-\infty}^{\infty}P_n^{\pm}R_n^{\pm}(z,z')\boldsymbol{j}_n(z')\mathrm{d}z'. \tag{12}$$

Here,

$$P_n^{\pm} = \begin{pmatrix} -\dfrac{\omega\mu_0 k_{y0}}{2\gamma_n k_n} & \dfrac{\omega\mu_0 k_{xn}}{2\gamma_n k_{zn}} & 0 \\ \pm\dfrac{k_{xn}}{2\gamma_n} & \pm\dfrac{k_{y0}}{2\gamma_n} & -\dfrac{\gamma_n}{2k_{zn}} \end{pmatrix}; \quad (13)$$

$$R_n^{\pm}(z,z') = \theta[\pm(z-z')]\exp[\pm\mathrm{i}k_{zn}(z-z')]; \quad (14)$$

$$\theta(z) = \begin{cases} 1, & z>0 \\ 1/2, & z=0 \\ 0, & z<0 \end{cases}; \quad (15)$$

δ_{nm} is the Kronecker symbol; $\gamma_n = \sqrt{k_{xn}^2 + k_{y0}^2}$.

The obtained relation (12) determines the basic solution of the generalised source method. Now we should derive expression (3) in the form suitable for further use. To do this, we will expand both sides of (3) in Fourier harmonics:

$$\boldsymbol{j}_n(z) = -\mathrm{i}\omega\{[\varepsilon(x,z) - \varepsilon_\mathrm{b}]\boldsymbol{E}(x,y,z)\}_n$$
$$= -\mathrm{i}\omega\sum_{m=-\infty}^{\infty}\varepsilon_{n-m}(z)\boldsymbol{E}_m(z) + \mathrm{i}\omega\varepsilon_\mathrm{b}\boldsymbol{E}_n(z)$$
$$= -\mathrm{i}\omega\varepsilon_\mathrm{b}\sum_{m=-\infty}^{\infty}\varDelta_{nm}(z)\boldsymbol{E}_m(z). \quad (16)$$

The convolution in (16) is represented in the form of a product of a Toeplitz matrix (i.e. a matrix whose elements only depend on the index difference) $\varDelta_{nm}(z)$ consisting of the Fourier harmonics of the permittivity and harmonics of the electric field components $E_{\alpha m}(z)$. Expressing in (16) the vector $\boldsymbol{E}_m(z)$ via (11), we obtain

$$j_{n\alpha}(z) = \sum_{m=-\infty}^{\infty}\sum_{\beta=x,y,z}V_{nm}^{\alpha\beta}(z)[Q_{m\beta}^{+}\boldsymbol{a}_m^{+}(z) + Q_{m\beta}^{-}\boldsymbol{a}_m^{-}(z)], \quad (17)$$

$$\alpha = x,y,z,$$

where $Q^{\pm}$ is the transfer matrix from the amplitudes of TE- and TM-polarised waves to the amplitudes of the electric field components,

$$Q_n^{\pm} = \begin{pmatrix} \dfrac{k_{y0}}{\gamma_n} & \dfrac{k_{xn}k_{zn}}{\omega\varepsilon_\mathrm{b}\gamma_n} \\ -\dfrac{k_{xn}}{\gamma_n} & \dfrac{k_{y0}k_{zn}}{\omega\varepsilon_\mathrm{b}\gamma_n} \\ 0 & \dfrac{\gamma_n}{\omega\varepsilon_\mathrm{b}} \end{pmatrix}, \quad (18)$$

and the components of the block-diagonal matrix V are expressed as

$$V_{nm}(z) = -\mathrm{i}\omega\varepsilon_\mathrm{b}\begin{pmatrix} \varDelta_{nm}(z) & 0 & 0 \\ 0 & \varDelta_{nm}(z) & 0 \\ 0 & 0 & \bar{\varDelta}_{nm}(z) \end{pmatrix}. \quad (19)$$

Here, $\bar{\varDelta}$ is the Toeplitz matrix with the coefficients expressed by the Fourier transforms of the inverse permittivity:

$$\bar{\varDelta}_{nm}(z) = \delta_{nm} - \varepsilon_\mathrm{b}\bar{\varepsilon}_{n-m}(z), \quad (20)$$

$$\bar{\varepsilon}_{nm}(z) = \frac{1}{\varLambda}\int_0^{\varLambda}\frac{1}{\varepsilon(x,z)}\exp[-\mathrm{i}(n-m)Kx]\mathrm{d}x. \quad (21)$$

As a result, substituting (17) into (12), we obtain

$$\boldsymbol{a}_n^{\pm}(z) = \delta_{n0}\boldsymbol{a}_\mathrm{inc}^{\pm}(z) + \sum_{\alpha=x,y,z}\int_{-\infty}^{\infty}\Big\{\sum_{m=-\infty}^{\infty}\sum_{\beta=x,y,z}P_{n\alpha}^{\pm}R_n^{\pm}(z,z')V_{nm}^{\alpha\beta}(z')$$
$$\times[Q_{m\beta}^{+}\boldsymbol{a}_m^{+}(z') + Q_{m\beta}^{-}\boldsymbol{a}_m^{-}(z')]\Big\}\mathrm{d}z'. \quad (22)$$

Expression (22) is an analogue of equation (4) of the generalised source method, as applied to the problem of electromagnetic radiation diffraction on a one-dimensional periodic plane structure. The implicit self-consistent equation (22), as will be shown in Section 3, allows one to construct the numerical algorithm in the form of a solution of the algebraic system of linear equations for which powerful and well-developed methods of linear algebra can be used.

Note that in deriving relation (19) for the V matrix, it was implicitly assumed that the index corresponding to diffraction orders ranges over an infinite number of values. However, in the course of numerical solution of the diffraction problem, only the finite number of the diffraction orders can be taken into account. The order number, on which the series of the finite sum is replaced, will be denoted by N_O. Then, for the case of diffraction gratings characterised by the discontinuous function $\varepsilon(x,z)$ (i.e., for profiled gratings), the function $\boldsymbol{E}(x,y,z)$ is also discontinuous in the spatial layer occupied by the grating, and the V matrix has the from different from (19) because the Fourier transform from the product of two discontinuous functions with the common points of discontinuity [see (16)] is not determined [19]. From these facts it transpires that if the points of discontinuity of two piecewise continuous functions (f and g) do not coincide, the series of products of their harmonics $\sum_{n=-N}^{N}f_{m-n}g_n$ is reduced to $\sum_{n=-\infty}^{\infty}f_{m-n}g_n$ at $N\to\infty$. However, if some points of discontinuity of the functions f and g coincide, it is necessary to calculate $\sum_{n=-N}^{N}[1/f]_{m-n}^{-1}g_n$ in order to correctly approximate the product fg by the Fourier series. Note that these rules should be also applied to the FMM. For quite a long time, this method neglected this rule, which was the reason for bad convergence of solutions for the TM-polarised wave diffraction. This fact was found experimentally in [7] and studied in [20, 21], as applied to the diffraction calculation on two-dimensional gratings.

To apply these rules, we will consider the fields at the grating profile interface separating different media. As is known, the tangential components of the electric field at this interface are continuous. Fourier series approximation of the product of the functions for these components does not require the matrix inversion and, hence,

$$(J_\parallel)_n = -\mathrm{i}\omega(D_\parallel - D_{\mathrm{b}\parallel})_n = -\mathrm{i}\omega\varepsilon_\mathrm{b}\sum_{m=-N_\mathrm{O}}^{N_\mathrm{O}}\varDelta_{nm}(E_\parallel)_m. \quad (23)$$

The normal vector component $\boldsymbol{D}$ on the grating surface is continuous; however, the corresponding component $\boldsymbol{E}$ has a discontinuity. Substituting $(1/\varepsilon)_{m-n}^{-1}E_n$ into (16) yields for the normal component of the generalised current $J_\perp$ the expressions:

$$(J_\perp)_n = -\mathrm{i}\omega(D_\perp - D_{\mathrm{b}\perp})_n$$
$$= -\mathrm{i}\omega\varepsilon_\mathrm{b}\sum_{m=-N_\mathrm{O}}^{N_\mathrm{O}}\Big(\frac{\bar{\varepsilon}_{n-m}^{-1}}{\varepsilon_\mathrm{b}} - \delta_{nm}\Big)(E_\perp)_m. \quad (24)$$

To use the relation between the generalised current and field (23) and (24), we should define the transformation of the coordinates, which expresses normal field and current components by their x-, y-, and z-components. Let the new coordinate system at each point of the interface between two media be introduced with the help of the inclination angle ψ to the z axis (Fig. 1). We will denote the axes of the new basis by p, y, q, the axis p being perpendicular to the interface between the media, while the axes y and q – parallel.

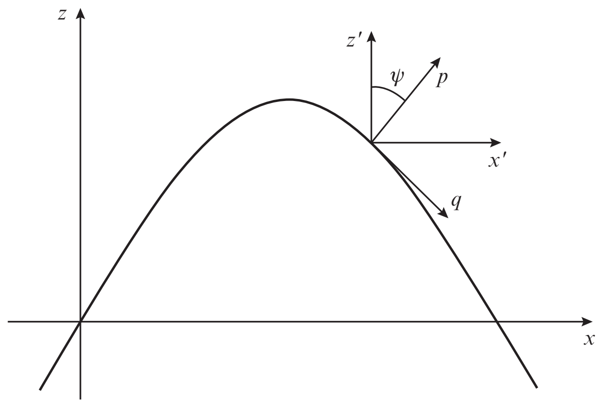

Figure 1. Local coordinate system on the grating surface.

We will assume below that the angle ψ is a smooth function. This is not a strong restriction because this function is in fact determined at some points on the x axis and thus can be extrapolated by a smooth function with a narrow spectrum. In this case, the Fourier transforms of the trigonometric functions of the angle ψ always exist, and the Toeplitz matrices corresponding to them are commutated with the matrices Δ_{nm} and $\bar{\Delta}_{nm}$. Thus, using (23), (24), and the matrix of rotation to the new coordinate system, we can obtain the relation between the field and the generalised current:

$$j_{n\alpha}(z) = -\mathrm{i}\omega\varepsilon_{\mathrm{b}} \sum_{\beta=x,y,z} \sum_{m=-\infty}^{\infty} [\delta_{\alpha\beta}\Delta_{nm}(z) + \Gamma_{\alpha\beta np}(z) D_{pm}(z)] E_{m\beta}(z), \tag{25}$$

where the tensor $\Gamma_{\alpha\beta}$ has four nonzero Toeplitz components: $\Gamma_{xxnm} = [\sin^2\psi]_{nm}$, $\Gamma_{zznm} = [\cos^2\psi]_{nm}$ and $\Gamma_{xznm} = \Gamma_{zxnm} = [\sin\psi\cos\psi]_{nm}$, while the matrix is

$$D_{nm}(z) = \frac{\bar{\varepsilon}_{nm}^{-1}(z) - \varepsilon_{nm}(z)}{\varepsilon_{\mathrm{b}}}. \tag{26}$$

Substitution of (25) into (10) yields

$$E_{nz} = -\sum_{m=-\infty}^{\infty} [\Gamma_{zx} CD]_{nm} E_{mx} + \sum_{m=-\infty}^{\infty} D_{nm} \tilde{E}_{mz}, \tag{27}$$

where

$$C_{nm} = \Big[\frac{\varepsilon_{nm}}{\varepsilon_{\mathrm{b}}} + \Gamma_{np} D_{pm}\Big]^{-1}. \tag{28}$$

Thus, using (25) and (27), for matrices $V_{nm}^{\alpha\beta}$ we obtain instead of (19) a new expression:

$$V_{nm}(z) = -\mathrm{i}\omega\varepsilon_{\mathrm{b}} \begin{pmatrix} \Delta_{nm} + [\Gamma_{xx} D - \Gamma_{xz}\Gamma_{zx} DCD]_{nm} & 0 & [\Gamma_{zx} CD]_{nm} \\ [\Gamma_{xx} D]_{nm} & \Delta_{nm} & 0 \\ [\Gamma_{zx} DC]_{nm} & 0 & \delta_{nm} - C_{nm} \end{pmatrix}. \tag{29}$$

Therefore, by applying the generalised source method, we have obtained equation (22) with the matrix $V_{nm}^{\alpha\beta}$ in the form of (19) for the case of continuously changing permittivity and in the form of (29) for the case of presence of an interface between different media.

3. Numerical solution

We will calculate the integral in equation (22) by dividing the plane layer with the diffraction grating into many sublayers. Let us denote their number by N_{L}. We assume that all the sublayers have the same thickness $\Delta h = h/N_{\mathrm{L}}$, and the amplitudes of plane harmonics have the values $a_{nq}^{\mathrm{e,h}\pm}$ at central points of the sublayers z_q, where the subscript n, as before, labels the diffraction orders and the subscript q – the sublayers: $q = 1, 2, ..., N_{\mathrm{L}}$, so that

$$z_q = z_0 + \Big(q - \frac{N_{\mathrm{L}} + 1}{2}\Big)\Delta h. \tag{30}$$

In addition, as was shown in the previous section, we will take into account the finite (from $-N_{\mathrm{O}}$ to N_{O}) number of diffraction orders. Then, equation (22) with the matrix V selected correspondingly will be reduced to a system of linear algebraic equations, making it possible to find the amplitudes of TE and TM harmonics in each sublayer:

$$\sum_q \sum_m A_{nmpq}^{\pm\pm} \boldsymbol{a}_{mq}^{\pm} = \sum_q \sum_m \Big(I_{nmpq}^{\pm\pm} - \sum_{\alpha=x,y,z} \sum_{\beta=x,y,z} R_{npq}^{\pm} P_{n\alpha}^{\pm} V_{nmq}^{\alpha\beta} Q_{m\beta}^{\pm} \Big) \boldsymbol{a}_{mq}^{\pm} = \delta_{n0} \boldsymbol{a}_{np}^{\mathrm{inc}\pm}, \tag{31}$$

where $I_{nmpq}^{\pm\pm} = \delta_{nm}\delta_{pq}\delta_{\pm eh}$ is a unit matrix. Matrices $I_{nmpq}^{\pm\pm}$ and $A_{nmpq}^{\pm\pm}$ can be treated as quadratic block matrices with $N_{\mathrm{L}} \times N_{\mathrm{L}}$ blocks, each of them containing $(2N_{\mathrm{O}} + 1) \times (2N_{\mathrm{O}} + 1)$ blocks of size 4×4.

The solution of the system of linear equations (31) allows one to directly calculate the amplitudes of diffraction harmonics on the plane layer and grating boundaries. Let us denote the z coordinates of the upper and lower boundaries of this layer by $z_1 = -h/2$ and $z_2 = h/2$, respectively. Then, from (22) and (31) we obtain

$$\boldsymbol{a}_n^{\pm}(z_1, z_2) = \delta_{n0} \boldsymbol{a}_n^{\mathrm{inc}\pm}(z_1, z_2) + \sum_q \sum_m \sum_{\alpha=x,y,z} \sum_{\beta=x,y,z} T_{nq}^{\pm} P_{n\alpha}^{\pm} V_{nmq}^{\alpha\beta} Q_{m\beta}^{\pm} (A_{nmpq}^{\pm\pm})^{-1} \times \delta_{m0} \boldsymbol{a}_{nq}^{\mathrm{inc}\pm}(z_1, z_2), \tag{32}$$

where $\boldsymbol{a}_n^{\pm}(z_1, z_2)$ is the amplitude vector of TE and TM harmonics at the layer boundaries; $\boldsymbol{a}_0^{\mathrm{inc}\pm}(z_1, z_2)$ is an analogous amplitude vector of the incident field; the matrix T describes the propagation of plane harmonics from each sublayer to the boundaries of the entire layer $z_{1,2}$. Its explicit form depends on the media surrounding the layer with a grating.

Recall that relations (31) and (32) are introduced under the following assumption: on both sides of the grating there is a medium with the permittivity ε_b. In this case, the matrix T has a simple form and its components can be written as

$$T^{+}_{nq} = \Delta h \exp[\mathrm{i}k_{zn}\Delta h(N_L + 1/2 - q)],$$
$$T^{-}_{nq} = \Delta h \exp[\mathrm{i}k_{zn}\Delta h(q - 1/2)]. \quad (33)$$

If the layer under study is between two different media with the permittivities $\varepsilon_{1,2}$, it is necessary to take into account additional waves emerging due to re-reflection from the layer boundaries. In this case, as is seen from the structure of the matrices entering equations (31) and (32), only the matrices R and T change. Let us denote the reflection and refraction coefficients for the waves incident from within the layer at the interface $z = z_1$ between the homogeneous media with the permittivities ε_1 and ε_b by $r^{\mathrm{e,h}}_{1n}$ and $t^{\mathrm{e,h}}_{1n}$ and at the interface $z = z_2$ by $r^{\mathrm{e,h}}_{2n}$ and $t^{\mathrm{e,h}}_{2n}$. Then, instead of expression (33) we should use expressions

$$T^{(\mathrm{e,h})(++)}_{nq} = \Delta h \frac{\exp[\mathrm{i}k_{nz}\Delta h(N_L + 1/2 - q)]}{1 - r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2k_{nz}h)},$$
$$T^{(\mathrm{e,h})(+-)}_{nq} = \Delta h \frac{r^{\mathrm{e,h}}_{1n}\exp[\mathrm{i}k_{nz}\Delta h(2N_L + 1/2 - q)]}{1 - r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2k_{nz}h)},$$
$$T^{(\mathrm{e,h})(-+)}_{nq} = \Delta h \frac{r^{\mathrm{e,h}}_{2n}\exp[\mathrm{i}k_{nz}\Delta h(N_L + q - 1/2)]}{1 - r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2k_{nz}h)},$$
$$T^{(\mathrm{e,h})(--)}_{nq} = \Delta h \frac{\exp[\mathrm{i}k_{nz}\Delta h(q - 1/2)]}{1 - r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2k_{nz}h)}. \quad (34)$$

The new expressions for the components of the R matrix describing the harmonic propagation between different sublayers take the form:

$$R^{(\mathrm{e,h})(++)}_{npq} = \Delta h\left[\theta^{+}_{p-q} + \frac{r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2\mathrm{i}k_{nz}h)}{1 - r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2\mathrm{i}k_{nz}h)}\right] \times \exp[\mathrm{i}k_{nz}\Delta h(p - q)],$$
$$R^{(\mathrm{e,h})(+-)}_{npq} = \Delta h \frac{r^{\mathrm{e,h}}_{1n}\exp[\mathrm{i}k_{nz}\Delta h(2N_L + 1 - p - q)]}{1 - r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2\mathrm{i}k_{nz}h)},$$
$$R^{(\mathrm{e,h})(-+)}_{npq} = \Delta h \frac{r^{\mathrm{e,h}}_{2n}\exp[\mathrm{i}k_{nz}\Delta h(p + q - 1)]}{1 - r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2\mathrm{i}k_{nz}h)},$$
$$R^{(\mathrm{e,h})(--)}_{npq} = \Delta h\left[\theta^{-}_{p-q} + \frac{r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2\mathrm{i}k_{nz}h)}{1 - r^{\mathrm{e,h}}_{1n} r^{\mathrm{e,h}}_{2n}\exp(2\mathrm{i}k_{nz}h)}\right] \times \exp[-\mathrm{i}k_{nz}\Delta h(p - q)]. \quad (35)$$

Thus, after determining all the matrices in expressions (31) and (32), it is necessary to construct an algorithm of their numerical solution. Note at once that the matrix size A can be very large (for example, at $N_O, N_L \propto 10^3$ the matrix size is $\propto 10^6$), which eliminates the possibility of its direct inversion. We solve the linear system (31) in this paper using the GMRES method because it has the best convergence among all the methods used to solve linear systems [14], which is critical in studying rather complex distributions $\varepsilon(x, z)$.

Each GMRES iteration contains one matrix-vector multiplication, which is the most time consuming part of the algorithm. In the general case, this operation requires $O(N^2)$ multiplication operations (N is the matrix size); however, expressions (31), (32) are constructed in such a way that it is possible to accelerate the execution of this operation. We used here the fact that the product of any Toeplitz matrix by the vector can be calculated with the help of the FFT during the time $O(N\log N)$ by 'stretching' the corresponding Toeplitz matrix into a circulant matrix [15]. Let us show that the matrix A is the product of only block-diagonal and Toeplitz matrices. The matrices P and Q are block-diagonal, which follows from (13) and (18). The matrix V is the Toeplitz matrix with respect to the subscripts pq because it consists of Fourier transforms of the permittivity and of the trigonometric functions of the angle ψ [see (19) and (29)]. The matrix R in the form (14) is also the Toeplitz matrix with respect to the spatial subscripts pq, which follows from its definition. In expressions for the modified matrix R (35), the first and the last submatrices have the Toeplitz structure. The second and the third matrices depend on the sum of the subscripts p and q but their product by the vector also can be represented in the form of a convolution by replacing the sign of one of the subscripts (in this case, the order of the elements should be inversed in the corresponding vectors and after multiplication they should be transformed backward).

Therefore, we obtain an iterative numerical algorithm based on the GMRES method in which the matrix-vector multiplications are calculated with the FFT. The method is fast and has a good convergence. For $(2N_O + 1)$ diffraction orders and N_L sublayers, the algorithm complexity can be estimated as $O\{(2N_O + 1)N_L\log[(2N_O + 1)N_L]\}$ [for large N_O and N_L, it can be treated as arbitrary close to linear with respect to the product $(2N_O + 1)N_L$]. Thus, the complexity of the method under study is significantly lower than that of the algorithm with the direct vector-matrix multiplication $O[(2N_O + 1)^2N_L^2]$ or than the FMM complexity $O[(2N_O + 1)^3N_L]$.

4. Numerical examples

As was mentioned in Introduction, there exist now several well-developed and widely used methods for calculating diffraction gratings. Therefore, within the framework of this paper we compare it with the FMM for diffraction on holographic and rectangular gratings and with the Rayleigh method for diffraction on sinusoidal gratings. All calculations were performed on a personal computer (2 GHz, 8 GB RAM). In comparisons, we studied the convergence of the solution while changing the number of layers into which the grating is divided. In this case, the number of diffraction orders is an additional parameter.

For all the calculations performed below, we used a grating with a period 1 μm and depth 0.5 μm, the wavelength of radiation incident at the angle 30° was 0.6238 μm. The error was determined as averaged absolute difference of the complex amplitudes of diffracted waves in the orders from –5 to 5. Figure 2 shows the solution convergence and its difference from the FMM solution during diffraction on the holographic grating specified by the dependence of the permittivity $\varepsilon(x) = 6.25(1 + 0.1\sin Kx)$ on the x coordinate. These dependences are almost unaffected by the number of the diffraction orders, which means that the solution obtained by

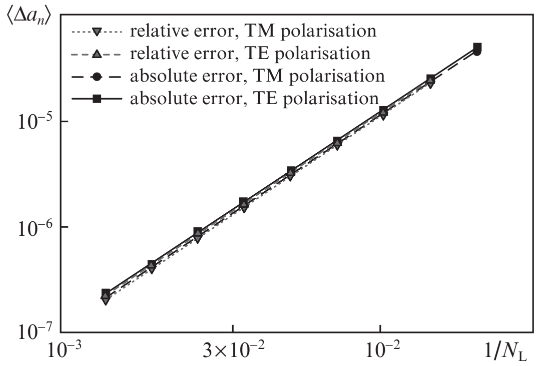

Figure 2. Convergence of the GSM (relative error) and its comparison with the FMM (absolute error) with increasing the number of layers in the grating. The permittivity of the substrate is equal to 6.25 and of the coating – to 1.

the proposed method coincides with the FMM solution in the limit of an infinite number of layers. A similar conclusion can be drawn by comparing the calculation results of diffraction on a rectangular grating (Fig. 3).

In the case of a sinusoidal grating, as is seen from Figs 4–6, the solution convergence weakly reflects the pure error. The comparison here was performed using the Rayleigh method, which gives an exact solution [12]. At each fixed number of diffraction orders and a sufficiently larger number of layers, the proposed method introduced some constant error, which decreases with decreasing the number of orders. Therefore, in the case of complex-shaped gratings, the accuracy, sufficient for practical use of the results, can be obtained when the number of diffraction orders exceeds 100.

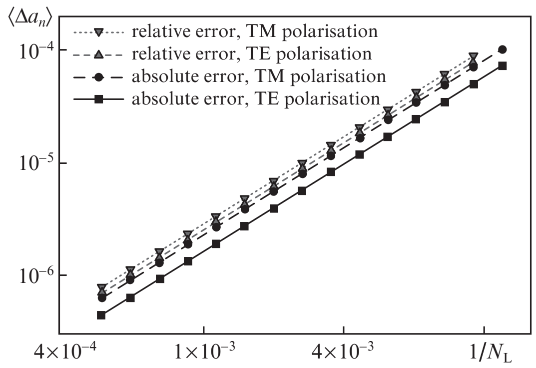

Figure 3. Same as in Fig. 2 but for a grating with a rectangular profile, the filling factor 0.5, and the permittivity 6.25.

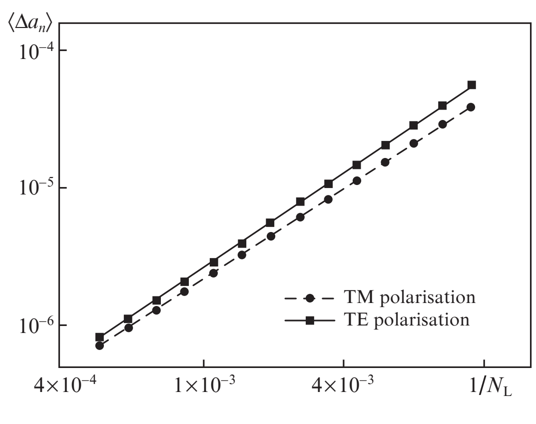

Figure 4. Convergence of the method in calculating the diffraction on a sinusoidal grating. The calculation parameters are the same as in the case of a rectangular grating (Fig. 3).

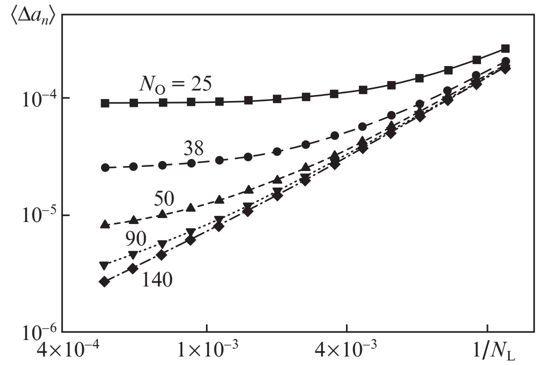

Figure 5. Comparison of the proposed method with the Rayleigh method during diffraction of a TE-polarised wave on a sinusoidal grating. Dependence of the averaged difference of solutions is presented for different numbers of diffraction orders used in calculations. The calculation parameters are the same as in the previous cases.

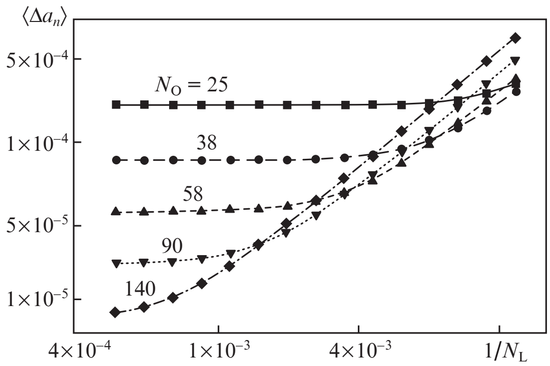

Figure 6. Same as in Fig. 5 but for TM polarisation.

The approximate number of GMRES iterations for a holographic grating is equal to 20, for a rectangular profile grating – to 50, and for a sinusoidal grating – to 150. The saving of the computation time compared to FMM for the above sinusoidal grating started with the matrix size for the GSM of the order of 10^5, the accuracy of both methods being 10^{-4}. This corresponds to approximately 50 diffraction orders and the grating division into 30 layers for the computation time ~15 s and 50 s for the TE- and TM-polarised diffractions, respectively. In the course of numerical simulation, we also found the following properties. At a sufficiently large number of diffraction orders, the number of layers should exceed the number of orders by 5–10 times to obtain the required accuracy. The thickness of one layer is, in this case tens, tens of a subnanometer or less. The required number of diffraction orders strongly depends on the grating period and the permittivity contrast; it increases with increasing these parameters. As a result, with the configuration similar to the above-mentioned, the personal computer can be used for calculating diffraction of the gratings whose depth and period are equal to several wavelengths and the contrast is approximately equal to that presented in the examples.

5. Conclusions

Thus, we have developed a new numerical method for calculating diffraction on dielectric gratings. The method can be treated as an alternative to the widely used FMM intended for calculating complex-shaped gratings. The FMM proves more preferable when the permittivity distribution is independent of the z coordinate because in this case the division of the grating into layers is not required. However, in the general case when this division is necessary, the efficiency of the proposed method increases with increasing the grating depth and period. Indeed, an increase in the grating depth requires an increase in $N_{\rm L}$, and the increase in the periods – an increase in $N_{\rm O}$; therefore, due to a smaller computational complexity the new method allows one to consider larger values of these parameters and thus gratings with a greater depth, period, and more complicated permittivity distribution. Provided the geometrical parameters of the gratings are decreasing, the proposed method, as the FMM, works the better the thinner the grating and the smaller the period and the contrast.

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