Modified integral method for weak convergence problems of light scattering on relief grating

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ABSTRACT

A rigorous modified integral method applicable for diffraction grating analysis working from x-ray - up to millimeter range is presented. The changes have been made both in theory, and in numerical realization. In theory special attention has been given to power balance criterion generalization for the case of absorbing gratings and to forms of Green's function representations. In comparison with the well known integral method formulated by Maystre, a lot of fundamental improvements have been made in the following numerical sections: the forms of representation of a groove profile, choice of points for calculation of unknown functions, integration method, choice of numbers of collocation points and Green's function expansion terms and their derivatives. For the first time stable convergence for all types of gratings and wavelengths, including those with very deep profiles, high conductivity, small wavelength-to-period ratios, and, especially, for TM polarization has been achieved and demonstrated. Examples of results are given for a wide range of transmission and reflection gratings and parameters of light. Diffraction efficiencies calculated with the help of the developed method of analysis are compared with published data and calculations performed by other researchers. All results have been obtained using ordinary PC and commercially available program PCGrate™ 2000X.

Keywords: integral method, PCGrate software, diffraction grating, electromagnetic theory, efficiency modeling, relief gratings, theory of grating, transmission gratings, reflection gratings, diffraction theory

1. INTRODUCTION

Among the large variety of rigorous theoretical approaches and their modifications used for calculation of diffraction efficiency of gratings, the integral equation method has a special place. First, it was one of the first numerical methods, with which help it was possible to solve important practical problems for periodic structures.[1] Second, it is the most universal and powerful tool for diffraction research on gratings of all types in wide spectral range until now, despite of very intensive development of other rigorous methods.[2,3] In many important cases the integral equation approach is a single known approach, acceptable from the practical point of view, for an accurate prediction of efficiency peculiarirties.[3-6] For this one has to pay in some complexity of the theory and various "subtleties" of numerical implementation, which are subjects of many researches, including this.

This work covers important features of the presented realization of integral method (which was named earlier "modified"[7]) and programs, developed on its basis, including commercial programs, in detail.[8] Using this approach the finite-difference integral equations have been deduced and a program taking into account all the best of integral method modifications, from the author's viewpoint, has been developed. This code including all proposed changes allows one calculate rigorously diffraction efficiency practically for all types of gratings in a very wide range of wavelengths from soft x-ray up to microwaves, even for the most difficult cases of weak convergence, which are described together with other examples of calculations in this work and quoted publications. All results are compared with approaches and data of other authors.

2. WHY MODIFIED?

Integral method applicable to diffraction periodic structures was well developed long ago. Here its basic moments are given which are necessary for full understanding of modified method, and also taking into consideration discrepancies and typing errors one can come across in the scientific literature. The comprehensible variant of the theory, with all final expressions necessary for code developments is presented. Those who are interested in details and history of the problem can be addressed to fundamental works.[1,9] As for the term "modified" integral method used by the author in publications, it applies, first of all, to a set of approaches of fundamental importance used in numerical implementation of the theory, and discussed hereinafter. Though, such important practical characteristics, to which special attention is also paid in this work, as generalization of power balance criterion for a case of absorbing gratings, or kinds of Green's function representations, apply directly to theory of integral method and deduction of integral equations. For achievement of good results, rigor

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and equation completeness, as well as uniqueness of integral equation solution are necessary, but, by far, not sufficient to obtain converging and steady efficiency values for many practical interesting cases. From this point of view, there is no distinct border between approach and technique of its realization. Those who even only once tried to solve diffraction problems by rigorous numerical methods, knows it for sure. Certainly, considerable progress in integral and other rigorous methods of grating efficiency calculation, achieved for last pair of decades, is due, first of all, to their numerical implementation techniques, and, also, to improvement of algorithms and computers.

3. DERIVATION OF INTEGRAL EQUATIONS

For brevity, derivation of integral equation is considered here only for a case when incident wave is polarized in the plane denoted TM or s (electric-field vector is in the plane, perpendicular to the grooves). Such polarization plane is chosen for two grounds. First, one seldom comes across description for this case in scientific literature, and, second, this case is usually more difficult for calculations, and namely obtaining convergent results for a number of difficult cases is major point of this work. Besides, results for TE polarization can be derived from similar expressions for calculation of unknown function (current density) for the TM case by simple substitution of one for the permittivity ratios, which are present in these expressions. More general case of arbitrary incidence angle named conical diffraction[1] and the case of multilayer gratings[6] can similarly be considered without special problems, at least, from the point of view of problem definition and derivation of integral equations.

Let the plane TM-polarized electromagnetic wave be incident from semi-infinite nonabsorbing space "+" on periodic relief boundary surface S (grating) of semi-infinite space "–", in general case, with finite conductivity. A line of intersection of this surface with plane XY is described by function f(x). The surface S is infinite in directions of X and Z axes, d - period, ϕ - angle of incidence (to axis OY), h - the depth of a groove, $\bar{n}$ - normal vector to the surface directed from "–" to "+". Inside of finite-conductive metal there is electromagnetic field satisfying to boundary conditions at surface S, and there is a current with finite current density. A plane electromagnetic wave with wave vector $\bar{k}^+$, lying, in our case, in plane XY, propagates from direction of "+" medium (y > 0). For this case a wave of arbitrary polarization can be represented by a sum of TE (p) and TM (s) polarized waves. There are only three components of the field (for a chosen plane of polarization they are H_z, E_x, and E_y), which satisfy homogeneous scalar Helmholtz equation for medium with electric permittivity ε and magnetic permeability of vacuum μ_0 (herein and hereinafter the case of not-magnetic media is considered):

$$\Delta U + k^2 U = 0, \qquad (2.1)$$

where U - any component field, and $k = |\bar{k}| = \omega\sqrt{\varepsilon}\sqrt{\mu_0}$, ω – cyclic frequency. Incident field $\bar{U}^i$ at point M(x, y) above the surface of the grating can be written in the form:

$$\bar{U}^i = \exp[ik^+(\sin(\phi)x - \cos(\phi)y)]\ \bar{e}_z, \qquad (2.2)$$

$k^+ = k_0\sqrt{\varepsilon^+} = 2\pi\sqrt{\varepsilon^+}/\lambda_0$, λ_0 - wavelength in vacuum, $\bar{e}_z$ - unit ort of axis Z. Herein and hereinafter the time factor $\exp(-i\omega t)$ is omitted.

For the basic types of polarization the diffracted field of the same polarization is formed as result of diffraction of incident wave in the space above the grating. For an incident field of arbitrary polarization, the polarization of diffracted field depends on the grating properties.[1] Total magnetic field in the space above the grating can be represented by the sum of incident field and diffracted field:

$$\bar{H} = \bar{H}^i + \bar{H}^d. \qquad (2.3)$$

Ii is possible to calculate diffracted field above a finite-conducting grating assuming that the identical field to can be produced by some current flowing in empty space on a surface, coinciding with the surface of the grating under consideration. Then, the diffracted field in the space above grating and its normal derivative can be expressed in terms of an unknown surface current. This enables one to consider the limit, to which the total field tends to when point of observation situated above the grating approaches medium interface. The limit values of the field and its normal derivative when point of observation approaches to this interface in lower medium are connected with the limit values of the field and its normal derivative in upper medium by boundary conditions. Using Helmholtz-Kirchhoff integral for the description of the field in lower medium one can derive the integral equation for a calculation of this unknown surface current.

For the case of TM polarization the electromagnetic field identical to the diffracted field, can be induced by fictitious magnetic surface current. This current density $\bar{j}_m$, designating current j_m , flowing through contour length unit of surface S on plane XY perpendicular to the contour can be given in the form of:

$$\bar{j}_m = j_m\delta(x - x')\delta(y - f(x'))\ \bar{e}_z, \tag{2.4}$$

where the product of Dirac delta functions $\delta(x - x')\delta(y - f(x'))$ is equal to 1 at $x = x'$ & $y = f(x')$ and is equal to 0 otherwise. The Maxwell equations for a field formed by this magnetic current in the upper space are given by:

$$\text{rot}\ \bar{E} = i\omega\mu_0\ \bar{H}; \qquad \text{div}\ \bar{E} = 0;$$
$$\text{rot}\ \bar{H} = \bar{j}_m - i\omega\varepsilon^+\ \bar{E}; \qquad \text{div}\ \bar{H} = 0. \tag{2.5}$$

It follows from these equations that the magnetic field amplitude satisfies the non-uniform scalar wave equation:

$$\Delta H + (k^+)^2 H = -i\omega\varepsilon^+ j_m \delta(x - x')\delta(y - f(x')). \tag{2.6}$$

The total field and, on the basis (2.3), the diffracted field satisfying equation (2.6) can be calculated as Helmholtz -Kirchhoff integral over unbounded surface S^+ taking into account the radiation condition:

$$H^d = \int_S{}^+ = \int_S \Gamma^+(x, y, s')\Phi(s')ds', \tag{2.7}$$

where s' - curvilinear coordinate along the profile line corresponding to rectangular coordinates $(x', f(x'))$, $\Phi(s') = -\omega\varepsilon^+ j_m\delta(x - x')\delta(y - f(x'))$. The elementary solution of Helmholtz equation, function $\Gamma^+(x, y, s'))$, is called Green's function of upper half-space.[1]

The integration over all surface S can be reduced to integration over one grating period, taking into account the quasi-periodicity of the incident field (2.2) and the diffracted field (2.7). This, the so-called Flocket condition, consists in that increment d of coordinate x results in multiplication of function H by $\exp(idk^+\sin(\phi))$:

$$H(x + d) = H(x)\exp(idk^+\sin(\phi)). \tag{2.8}$$

Therefore, integral in (2.7) can be considered as the sum of integrals over infinite number of grating periods, and Green's function for upper half-space can be represented as infinite series with respect to n:

$$\Gamma^+(x, y, s')) = (-i/4)_{n=-\infty}\Sigma^\infty H_0^{(1)}[k^+((x - x' - nd)^2 + (y - f(x'))^2]^{1/2}\exp(indk^+\sin(\phi), \tag{2.9}$$

where $H_0^{(1)}$ - Hankel function[10] of order zero of the first kind. The Green's function in (2.9) represents radiation function of infinite set of filament sources, equally spaced from one another at a distance of d, the radiation phase of which is taken into account by an exponential factor. Zeroth term of this series takes into account at the point of observation (x, y) contribution of the section of a surface located near to a point $(x', f(x'))$ within the limits of one period of the grating, over which the integration is made. All other terms take into account contributions of the similar sections located in other periods of the grating to the left and to the right of the period of integration. Thus, integral over one period is equivalent to the integral over all surface S.

The sum of cylindrical functions of radiation is equivalent to the sum of plane waves. With help of the Poisson summation formula, the Green's function can be given in another form - in the form of expansion into series of plane waves:

$$\Gamma^+(x, y, s') = [_{-\infty}\Sigma^\infty (\exp(i\alpha_n(x - x') + i\gamma_n^+|y - f(x')|)/\gamma_n^+]/(2id), \tag{2.10}$$

where $K = 2\pi/d$, $\alpha_n = nK + \alpha_0$, $\alpha_0 = k^+\sin(\phi)$, $\gamma_n^+ = [(k^+)^2 - \alpha_n^2]^{1/2}$ - y-components of wave vectors. At $y > f_{max}(x')$ the waves which are included in expansion into series (2.10) have the same components of wave vectors, as the waves forming Rayleigh expansion[1] of the diffracted field.

The convenience of use of one of the equivalent Green's function (and their derivative) representation forms depends on interesting asymptotics and accuracy of calculations, the topics discussed below. In case of high-conductive metal and fast wave attenuation in it, the Green's functions of the medium can be calculated using expansion (2.9) in series of Hankel functions, and the derivative - using series obtained from (2.9) by differentiation. In work[1] only zeroth term of such series has been taken into account and its asymptotic has been calculated for an argument tending to zero. Such method of calculation neglects interference of points of the surface, which are located in adjacent sections of partition. The numerical investigations have shown, that such assumption is correct only for very high conductivity, inherent to metals in the middle and far IR range. In the UV, Visual and near IR range one has to take into account the interference of points. Therefore, it is not enough to have Hankel functions asymptotics for calculations of Green's function and its of derivative for metals. In this work expansion of type (2.10) has been used, and number of terms has been optimized when necessary.

With the regard for Flocket condition and relation $ds' = (1 + f'(x'))dx'$, integrands in (2.7) can be replaced with new integrands as follows:

$$\Psi(x', f(x')) = \Phi(x', f(x'))\exp(-i\alpha_0 x')(1 + (f'(x'))^2)^{1/2};$$
$$G^+(x, y, s') = \exp(i\alpha_0 x)[{}_{-\infty}\Sigma^{\infty} (\exp(iKn(x - x') + i\gamma_n{}^+|y - f(x')|)/\gamma_n{}^+]/(2id). \quad (2.11)$$

Now integral (2.7) can be represented as integral over one grating period:

$$H^d = \int_d G^+(x, x', y, f(x'))\Psi(x', f(x'))dx'. \quad (2.12)$$

In the case of TM polarization, the integral in (2.12) describes tangential component of the magnetic field, that on the surface itself, on which fictitious magnetic current flows, must be continuous. Therefore, while point M(x, y) is crossing surface S the field described by integral (2.12), must be continuous. It actually takes place, as the logarithmic singularity of the Green's function, present in (2.12) at x = x ' and y = f(x'), is integrable. The total field (2.3) in all space is equal to the sum of fields, one of which is defined by integral (2.12), and the other is falling down (2.2). Thus, the limit value of the tangential component of the total field H^+ for the point of observation M(x, y), moving above the grating to a point (x, f(x)) at surface S, is equal to the value of the total field at this point:

$$H^+(x, f(x)) = H^i(x, f(x)) + \int_d G^+(x, x', f(x), f(x'))\Psi(x', f(x'))dx', \quad (2.13)$$

In the case of TM polarization a normal derivative of the magnetic field is proportional to a tangential component of electrical field (2.5), for which, in the presence of surface magnetic current, the following boundary condition must be carried out:

$$E_t^+ - E_t^- = j_m. \quad (2.14)$$

Hence (2.5), for the break of normal derivative of the magnetic field, a break condition is satisfied as follows:

$$(dH/dn)^+ - (dH/dn)^- = -i\omega\varepsilon^+ j_m. \quad (2.15)$$

Differentiation of expression (2.13) along normal gives half-sum of field normal derivative limit values, which are obtained at approach of point of observation M(x, y) to a point of the surface from below and from above:

$$((dH/dn)^+ + (dH/dn)^-)/2 = dH^i(x, f(x))/dn + \int_d(dG^+(x, x', f(x), f(x'))/dn')\Psi(x', f(x'))dx'. \quad (2.16)$$

From here, using (2.12) and (2.15), an expression for field normal derivative limit value, at approach of point of observation M(x, y) to a point of surface S from above, is obtained:

$$(dH(x, f(x))/dn)^+ = dH^i(x, f(x))/dn + 0.5\Psi(x', f(x'))\exp(i\alpha_0 x')/(1 + (f'(x'))^2))^{1/2}$$
$$+ \int_d(dG^+(x, x', f(x), f(x'))/dn')\Psi(x', f(x'))dx'. \quad (2.17)$$

Thus, the value of the total field and its normal derivative in the upper medium and on the surface boundary of medium proves to be expressed by one unknown scalar functions Ψ. The diffracted field is calculated by formula (2.12). Green's function normal derivative, included in the expression (2.16) and (2.17) is defined as follows:

$$dG^+(x, x', y, f(x'))/dn' = {}_{-\infty}\Sigma^{\infty}\exp(i\alpha_0 x)/(2d(1 + f'(x'))^2)[\mathrm{sign}(f(x) - f(x')) - f'(x')\alpha_n/\gamma_n{}^+)$$
$$\times \exp(iKn(x - x') + i\gamma_n{}^+|f(x) - f(x')|], \quad (2.18),$$

where the sign function sign(f(x) – f(x')) is equal 1, if (f(x) – f(x')) ≥ 0, and –1 - otherwise.

Using the boundary conditions on the surface it is possible to determine values of the field and its normal derivative on the same surface in the lower medium. In the case of TM polarization, value of the field on the boundary in the lower medium is equal to the corresponding value of the field in upper medium, and normal derivative value is calculated according to boundary condition (2.24). If one considers all space as space filled with substance, then knowledge of a values of the field and its normal derivative in this substance on the surface coincident with initial boundary surface of media, allows one to describe the field under the surface with the help of Helmholtz-Kirchhoff integral also. At that, in the lower medium the incident field is absent. In dielectrics there is a finite number of propagating harmonics which satisfy to the radiation condition, and in absorbing medium all existing waves are fading while moving off from the boundary in the direction of negative values of y. Therefore, if for a closed contour of integration is chosen a contour, adjoining to the line of crossing S with plane XY, and closed at $y \to -\infty$, then the contribution to Helmholtz-Kirchhoff integral along contour part, which is infinitely far removed in direction y, is equal to zero, and all integral along the closed contour is equal to the integral along part of the contour, adjoining to surface S. Green's function and its normal derivative in this integral are represented by expressions similar of those used for the upper space in (2.11) and (2.18). They are obtained by replacement of values $\gamma_n{}^+$ with corresponding values $\gamma_n{}^-$ for the substance under consideration:

$$\gamma_n^- = ((k^-)^2 - \alpha_n^2)^{1/2},\ \mathrm{Im}\,(\gamma_n^-) > 0;\ \mathrm{Im}\,(\gamma_n^-) = 0,\ \mathrm{Re}(\gamma_n^-) > 0 \qquad (2.19)$$

where $k^- = k_0\sqrt{\varepsilon^-}$, ε^- – electric permittivity of the lower medium.

The integral equations for function Ψ are obtained on condition that in the integral under consideration the point of observation moves from the lower medium on the surface of integration. Using expressions (2.12) and (2.16), and, also, the considered boundary conditions, the integral equation for determination of unknown function Ψ is finally obtained:

$$H^i(x)/2 + \int_d [(\varepsilon^-/\varepsilon^+)G^-(x, x')dH^i(x')/dn' + H^i(x')dG^-(x, x')/dn']dx' = -0.5(\varepsilon^-/\varepsilon^+)\int_d G^-(x, x')\Psi(x')dx'$$
$$- 0.5\int_d G^+(x, x')\Psi(x')dx' - \iint_d [G^+(x', x'')dG^-(x, x'')/dn'' - (\varepsilon^-/\varepsilon^+)G^-(x, x'')dG^+(x', x'')/dn'']\Psi(x')dx'dx'', \qquad (2.20)$$

where G^- - Green's function for the lower medium, and dG^-/dn' and dG^-/dn'' are taken positive.

The amplitudes of the diffraction orders of number n in the upper medium can be obtained from (2.12) and Rayleigh expansion[1] for plane waves equating coefficients for the corresponding harmonics:

$$A_n^+ = -0.5i/(d\gamma_n^+)\int_d[\exp(-i\gamma_n^+ f(x') - inKx')\Psi(x', f(x'))]dx'. \qquad (2.21)$$

In practice, absolute diffraction efficiency of the grating E_n^+ is an important value. It is defined as a value of the energy flux, going off from the grating in the n-th order, per unit of the incident energy flux flow. Then, for y-component of Umov-Poynting vector we have:

$$E_n^+ = |A_n^+|^2\gamma_n^+/\gamma_i. \qquad (2.22)$$

The amplitude of the field and its normal derivative in the lower medium can be found from expressions similar to (2.13) and (2.17), as a limit at approach of a point of observation from below to the boundary surface S, taking into account the expression for the diffracted field (2.12) on the boundary surface and boundary conditions. The boundary conditions in the TM case of polarization are expressed in a continuity of the field on the boundary and in a jump of its normal derivative:

$$(dH/dn)^+/(dH/dn)^- = \varepsilon^+/\varepsilon^-. \qquad (2.24)$$

Taking this into account, we obtain:

$$H(x, f(x)) = H^i(x, f(x)) + \int_d G^+(x, x', f(x), f(x'))\Psi(x', f(x'))dx', \qquad (2.25)$$
$$(dH(x, f(x))/dn)^- = (\varepsilon^-/\varepsilon^+)[dH^i(x, f(x))/dn + 0.5\Psi(x', f(x'))\exp(i\alpha_0 x')/(1 + (f'(x'))^2)^{1/2}$$
$$+ \int_d(dG^+(x, x', f(x), f(x'))/dn')\Psi(x', f(x'))dx']. \qquad (2.26)$$

Amplitude of the n-th diffraction order in the lower medium can be expressed with the help of expressions (2.25) and (2.26):

$$A_n^- = (-0.5/d)\int_d\{[(-1 - f'(x')\alpha_n/\gamma_n^-)H(x', f(x')) + (dH(x', f(x'))/dn)^-/(i\gamma_n^-)]\exp(i\gamma_n^- f(x') - inKx')\}dx'. \qquad (2.27)$$

In the case of dielectric lower medium, the diffraction efficiency for n-th order is calculated as follows:

$$E_n^- = |A_n|^2\gamma_n^- \sqrt{\varepsilon^+}/(\gamma_i\sqrt{\varepsilon^-}). \qquad (2.28)$$

On the basis of Umov-Poynting theorem it is also possible to determine energy W_A, absorbed by material of the grating per unit of time. It is equal to the integral for the normal component of energy flux density $\bar{w}^-$, calculated on the lower closed surface S^-:[11]

$$W_A = \int_{S^-} = \int_S \bar{w}^-\ \bar{n}\ ds', \qquad (2.29)$$

where $\bar{w}^- = \bar{E}^- \times \bar{H}^-$ - Umov-Poynting vector in the lower medium. Taking into account (2.5), quasi-periodicity of the field, and, also, the complex valued amplitudes and their normal derivatives, it is not difficult to obtain value W_A averaged over time:

$$E_A = 0.5\int_d \mathrm{Re}[(dH/dn)^- H^{*-}/(i\omega\varepsilon^-)]ds', \qquad (2.30)$$

where H^{*-} - conjugate complex value of a field amplitude in the lower medium, $(dH/dn)^-$ - normal derivative of a field amplitude in the lower medium.

Normalized to unit of incident field energy flux, the value E_A, added to the sum of all propagating harmonics efficiencies E_n, expresses nothing else but the energy conservation law for gratings and generalizes it for the case of finite conductivity. Together with the reciprocity theorem, the compliance of infinite conducting and dielectric gratings with this law is always one of the basic criteria for testing correctness and reliability of developed programs[1]. Now, with the help of simple and natural definition (2.30) of physical quantity E_A, it can be also used for the most important case of finite conducting gratings with the same degree of rigour (namely, for sufficiently smooth surfaces[10]). The author for a long time[12] has been applying this useful generalization of the energy conservation law to calculations for absorbing gratings with any relief profile and never had grounds for doubts about correctness of its introduction. Use of E_A will be illustrated further with numerical examples.

4. FEATURES OF NUMERICAL REALIZATION

The solution of the integral equations is obtained by a known point matching method (collocation method), based on replacement of an integral equation by system of linear algebraic equations. It assumes a finding of N values of unknown quasi-periodic function Ψ, which can be approximated by step function in N points of one grating period. At the same time, certain requirements for continuity and smoothness of functions Ψ and f(x)[1] are imposed. Solution of a system of N linear equations in N unknowns by such method is, in general, incorrect. At the approximate numerical solution of integral equations reducing them to a truncated system of linear algebraic equations, we obtain an ill-conditioned system, all matrix elements of which have identical order of magnitudes. This is the major source of errors and it must be taken into account at construction of numerical algorithm.

For the integral equation of the first kind there is a logarithmic singularity in its kernel,[1] that is square integrable. However, for this reason the diagonal matrix elements of algebraic system are greater than off-diagonal elements. This forms a basis for self-regulation realization[13] for the Fredholm integral equation of the first kind such as (2.20). Construction of an effective algorithm for Green's function calculation is based on extraction of logarithmic singularity in an explicit form.[1-3,6,9] Often an accuracy of obtained results and the calculating time of task depend on correct account of Green's function singularity. However, as show numerical researches of the author, such specification is not always justified, (e.g. for some problems due to particularities of integrand numerical calculations (see below), for sufficiently high values of N) and requires separate research. Kernel of integral equation of the second kind at coincidence of an argument has removable singularity and it does not require of special extraction of this singularity at numerical realization. At that, the system is frequently ill-conditioned, as in some examples given below.

Let's divide contour f(x) by points x_k, k = 0;N, $x_0 = x_N$ into N parts. Function $\Psi(x_k, f(x_k))$ on each interval $[x_k, x_{k+1}]$ is considered to be constant. At that, integral equations (2.20) are reduced to a system of linear algebraic equations like this:

$$0.5\Psi(x_j, f(x_j)) + {}_{k=0}\Sigma^{N-1} c_{jk}\Psi(x_k, f(x_k)) = b(x_j, f(x_j)), \; j = 1, N. \qquad (3.1)$$

Let's make the solution at N midpoints of intervals $[x_k, x_{k+1}]$ and replace integrals over all period in (3.1) with the sums of integrals over intervals. These integrals are calculated with good approximation for some N and an appropriate choice of integration method. For more accurate approximation to sought function by mesh function it is desirable to choose interval $[x_k, x_{k+1}]$ small enough to enable calculations for quickly varying functions. On the other hand, the account of kernel singularities in integral equation (2.20) and necessity of obtaining a well-conditioned matrix in system (3.1) require one to choose an integration step large enough. Here we come, perhaps, to the most important point connected with use of a suitable integration method. As shown in work[1], in case of regular kernel and periodic integrand function in the right part, which takes place in (2.20), a step function approximation of integrand expression, with division of integration interval (period) into equal parts, is preferable. Such method of integration is mentioned as rectangle rule or trapezium rule, what, in this case, is equivalent. Indeed, this simple approach gives good results for many applications. However, in the most difficult cases its use does not produce good convergence of computed results even for very large N (about one thousand and more). First of all, efficiency calculations for the following types of gratings: very deep, deep with vertical slopes of a groove profile, deep high-conductive, deep with the small wavelength-to-period ratio, with the arbitrary (real) form of groove profile, and also echelle are related to such cases. It is especially correct for TM polarization and near to various kind of anomalies.[14] For improvement of integration accuracy, one can try to divide the profile by points set along axis X non-uniformly to increase their density near the edge or on the abrupt side, but it is not clear according to what law it must be done to integrate with high accuracy the periodic integrand expression. Until now, any acceptable decision is not known on this way.

The other approach follows from the integral equation for of diffracted field (2.7) itself - integration along arc length of contour f(x). But its difficulty consists in impossibility, for an arbitrary contour, to express coordinates of its points through arc lengths. Fortunately, for gratings, approximated by intervals of straight lines, it is not a problem. In this case, coordinates of surface points, are easily calculated by simple dividing of coordinate on axis X by cosine of inclination of the interval, and curvilinear integral along arc length is replaced usual. For a long time (at least, since work[15]), the author has been using this approach for solution of, practically, any diffraction problems for gratings for several reasons. First, it is almost as simple, as approach[1], but with far better results for the difficult cases described above. Second, it is equivalent to approach[1] for symmetric profiles and profiles with vertical slopes, and, asymptotically, transforms at decreasing depth and steepness of a profile into the approach,[1] and can be successfully used equally with it for calculation of any shallow and flat gratings. At last, third, it allows one to calculate very accurately the efficiencies of gratings, which profile has been measured earlier by any experimental technique: with help of AFM, STM, SEM, interferometer of high magnification, Talystep & other,[16-19] and relief of groove profile has been represented by real points, instead of using its Fourier expansion.[1]

On the basis of aforesaid, the integrand expression in (2.20), taken at the midpoint of interval Δx_k, is factored outside the integral sign and multiplied by interval length equal to:

$$\Delta x_k = x_{k+1} - x_k = d/(N\cos(\theta_k)), \tag{3.2}$$

where θ_k - inclination of an element of groove profile. At that, the matrix elements of equations (3.1) look like:

$$c_{jk} = -\,0.5\Delta x_k\{(\varepsilon^-/\varepsilon^+)G^-(x_j, x_k) + G^+(x_j, x_k) + 2\Delta x_k \,{}_{l=0}\Sigma^{N-1}[G^+(x_{l+1/2}, x_k)dG^-(x_j, x_{l+1/2})/dn_{l+1/2}) - (\varepsilon^-/\varepsilon^+)G^-(x_j, x_{l+1/2})dG^+(x_{l+1/2}, x_k)/dn_{l+1/2}]\}. \tag{3.3}$$

The free term of the equation (3.1) looks like:

$$b(x_j) = 0.5H^i(x_j) + {}_{k=0}\Sigma^{N-1}[(\varepsilon^-/\varepsilon^+)G^-(x_j, x_k)dH^i(x_k)/dn + (dG^-(x_j, x_k)/dn_k)H^i(x_k)]\Delta x_k. \tag{3.4}$$

The Green's functions and their derivatives for the upper and the lower half-space are calculated similarly, according to (2.11), (2.18) and (2.19):

$$G^{\pm}(x_j,x_k) = {}_{n=-P\pm}\Sigma^{P\pm}\{(\gamma_n^{\pm})^{-1}\exp[i\gamma_n^{\pm}|f(x_j) - f(x_k)| + inK(x_j - x_k)]\}, \tag{3.5}$$

$$dG^{\pm}(x_j, x_k)/dn_{j,k} = (2d)^{-1}\,{}_{n=-M\pm}\Sigma^{M\pm}[\mathrm{sign}(f(x_j) - f(x_k)) - f'(x_{j,k})\alpha_n/\gamma_n^{\pm}]\exp[i\gamma_n^{\pm}|f(x_j) - f(x_k)| + inK(x_j - x_k)], \tag{3.6}$$

where j, k = j - for the upper medium, and j, k = k - for the lower medium.

As follows from (2.7), the contribution of portions of surface S is proportional to both current values on these portions, and Green's functions. Interference of portions the weaker, the farther they are from one another on surface S. Therefore, there is no necessity for infinite limits of integration to obtain a sufficient accuracy of calculations of the integrals in (2.7) in the fixed point of observation. The limitation of numbers of series terms (3.5) and (3.6) for the lower and the upper medium, correspondingly, by $P^{\pm}$ and $M^{\pm}$, means, for integration, the limitation of number of the grating periods, which interference contribution must be taken into account to obtain necessary accuracy of calculations. However, values of $P^{\pm}$ and $M^{\pm}$ can not be more, than N, as, then, the matrix elements in (3.3) begin to diverge. In general, all these numbers must be optimized for each specific case. The rule proposed in[1] $P^{\pm} = M^{\pm} = 2N/3$ is far from being optimal for many cases and depends on specific numerical realization. For usual cases of calculations, more optimal "golden" rule is proposed in the present realization of integral method:

$$P^{\pm} = M^{\pm} = P = N/2. \tag{3.7}$$

For obtaining $(N+1)^2$ coefficients of system (3.1) one must execute number R of complicated operations with complex exponential functions:

$$R = (N+1)^2P. \tag{3.8}$$

Therefore, a choice of P for the benefit of a smaller number is very important during realization of long calculations. At that, it is naturally supposed, that values coincide with required accuracy. As for considered difficult cases, for some of them this "golden" rule serves very well, but other cases need optimization of parameter P (see Sections 5, 6). Fortunately, for the considered examples, optimization of $P^{\pm}$ and $M^{\pm}$ was never required.

Incident field and its normal derivative are calculated in accordance with (2.2) by the expressions:

$$H^i(x_k) = \exp(-i\gamma_i f(x_k)), \tag{3.9}$$

$$dH^i(x_k)/dn = -i(\gamma_i + \alpha_0 f'(x_k))\exp(-i\gamma_i f(x_k)). \tag{3.10}$$

Set N of numbers $\Psi(x_k)$, which are the solutions of the system of algebraic equations (3.1), allow one to calculate values of a surface magnetic field and its normal derivative (2.25, 2.26):

$$H(x_k) = H^i(x_k) + \Delta x_k \,{}_{l=0}\Sigma^{N-1}G^+(x_k, x_l)\Psi(x_l), \tag{3.11}$$

$$(dH(x_k)/dn)^{\pm} = (\varepsilon^-/\varepsilon^+)[dH^i(x_k)/dn + \Psi(x_k)/2 + \Delta x_k \,{}_{l=1}\Sigma^{N-1}\Psi(x_l)dG^{\pm}(x_k, x_l)/dn_k], \tag{3.12}$$

where $\varepsilon^-/\varepsilon^+ = 1$ for the upper half-space.

The amplitude of the n-th diffraction order propagating above and under the grating, is calculated according to (2.21) and (2.27):

$$A_n^+ = \Delta x_k/(2id\gamma_n^+)_{\kappa=0}\Sigma^{N-1}\exp(-i\gamma_n^+ f(x_k) - inKx_k)\Psi(x_k), \qquad (3.13)$$

$$A_n^- = \Delta x_k/(2d)_{\kappa=0}\Sigma^{N-1}[(1 + \alpha_n f'(x_k)/\gamma_n^-)H(x_k) + (i\gamma_n^-)^{-1}(dH(x_k)/dn)^-]\exp(i\gamma_n^- f(x_k) - inKx_k). \qquad (3.14)$$

Corresponding efficiencies of the orders are obtained from (2.22) or (2.28), and the absorption is obtained from (2.30):

$$E_A = {}_{\kappa=0}\Sigma^{N-1}\mathrm{Re}[(dH(x_k)/dn)^- H^*(x_k)/(2i\omega\varepsilon^-)]\Delta x_k. \qquad (3.15)$$

5. CONVERGENCE OF CALCULATIONS

A difficult enough and interesting example from work[20] has been chosen for demonstration of convergence of the obtained implementation of the modified integral method on optimization parameter P (number of Green's function expansion terms) and truncation parameter N (number of collocation points). A triangular metal grating with a vertical facet, electric permittivity of metal $\varepsilon^- = -21 + i.60.4$, depth equal to the grating period, and $\lambda/d = 0.7$ has been illuminated by TM-polarized wave at angle 25° with respect to the flat facet. In Fig.1 the convergence of efficiency calculation results for three orders (0, –1 and –2) and total energy balance for number P is shown at the values of truncation parameter N equal to 100, 300 and 500. It is evident the results converge for all three values of N at value of parameter P, close to 100% relative to N. For P, according to a "gold" rule (P = N/2), the efficiency values and the balance are still far from converging values. At first, the convergence is fast and oscillating and then, after reaching monotonous part of the curve, it is slow, but stable. The spread in values is the less, the higher truncation parameter N.

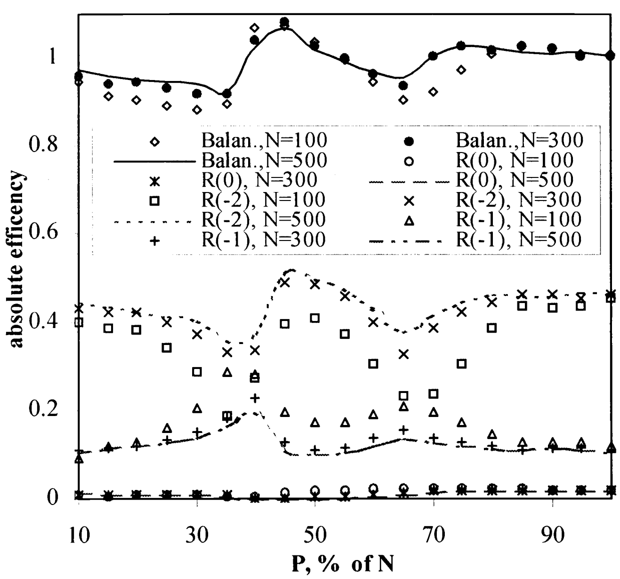

Fig.1. Absolute efficiency in 0, -1 and -2 orders and balance of a grating from,[20] as a function of P for N = 100, 300, 500.

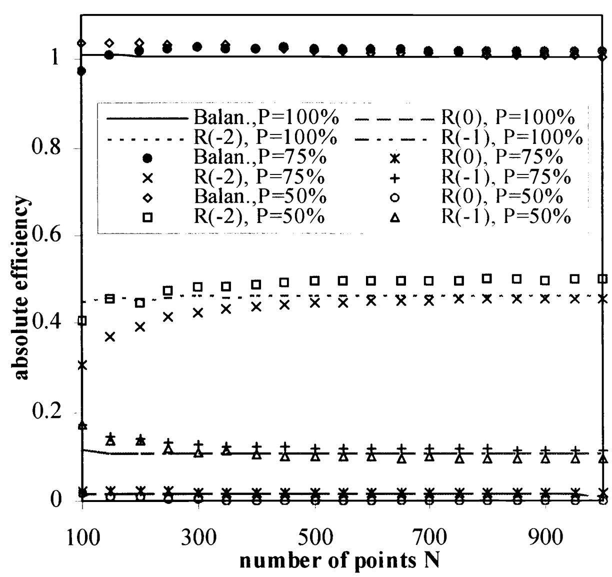

Fig.2. Absolute efficiency in 0, -1 and -2 orders and balance of a grating from,[20] as a function of N for P = 50, 75, 100%%.

The above mentioned statements are proved by dependence for efficiency values on truncation parameter N, presented in Fig.2. The curve for P = 100% (P = N) is changing monotonously and very slowly with increasing N from 100 to 1000, i.e. by one order. The relative error for N = 100, in comparison with values obtained for N=1000, makes up several percents for absorption and all the orders, except for the 0-th order, and 7% for this low efficiency order. Approximately, the same difference (see column 3 in Table 2) is observed comparing to work[20] and it tends to decrease with increasing N. Thus, the convergence for truncation parameter N is very fast for this example for the chosen optimum value P. For P = 75% convergence is good, but slower, than for P = 100%. For P = 50% the convergence also takes place, but it is much worse, than in case of the optimum P, especially, for the 0-th order. Therefore, in similar cases, it is more efficient to optimize at first parameter P for small N, and, then, to calculate efficiency with required accuracy for N with the obtained P.

It is interesting to note, that in the examples, considered below, optimization of parameter P is required in single case, also for an asymmetric triangle (see column 2 in Table 3). In that example the optimum P makes up only 10% because of high conductivity of a grating material and small ratio $\lambda/d = 0.1$.

6. EXAMPLES OF CALCULATIONS FOR DIFFICULT CASES

To show opportunities of the modified integral method and programs, created on its basis, including commercial ones,[8] a number of examples difficult for calculations have been chosen for deep and super-deep transmission and reflection gratings. These calculations are really difficult, and until to-day many of them are hard to fulfill for integral and other rigorous methods.[2] All results obtained here, are compared with the published data and calculations, kindly performed by the professor Lifeng Li. The modeling of efficiency has been carried out on a PC with Intel™ Pentium III 733 MHz processor, 256 KB Cash and 128 MB of RAM, working under MS™ Windows NT, v. 4.0. All results have been obtained with the help of the commercially available program PCGrate™ 2000X,[8] written on programming language C++.

In Tables 1-3 the calculation efficiency results for dielectric and metallic gratings for the various groove profiles with depth up to h/d = 10 and parameters corresponding to a wide range of spectrum from VUV to middle IR are given (positive incident angle is on the left of the normal). Now, from the point of view of the theory, as deep gratings are considered those with depth of about grating period, and as very deep gratings - those with depth of several periods and, even, ten or more periods. The modern state of technology, in principle, already provides manufacturing of very deep gratings of spectroscopic quality.[2] Before the present work, such deep gratings have been considered not to be analyzed by any integral method.[21-24]

The results of calculations for dielectric gratings, basically, for TM polarization, are given in Table 1. As examples of calculations, the author presents more gratings with a vertical facet of a groove profile (lamellar and asymmetrical triangular with left angle θ_1 and right angle θ_2) for two reasons. First, one meets this type of a profile more often in the publications about very deep gratings. Second, not all values obtained in[21] by modal method for the sinusoidal gratings are accurate enough. For instance, for TM polarization, the author[21] used only 10 partitions for representation of sinusoidal profile by rectangular layers at ratio h/d = 1 for a metallic grating.

Table 1. Diffraction efficiencies of various deep and very deep dielectric gratings, %.

Order	Sinusoidal, $d/\lambda=1.7$, h/d=1, TM pol., $\phi=30°$, $\varepsilon^+=1$, $\varepsilon^-=2.25$,			Triangle, $d/\lambda=1$, h/d=2.1, $\theta_2=90°$, $\phi=30°$, $\varepsilon^+=1$, $\varepsilon^-=2.5$			Triangle, $\lambda/d=0.7$, TM pol., h/d=1.0, $\theta_2=90°$, $\phi=25°$, $\varepsilon^+=1$, $\varepsilon^-=2.25$			Lamellar, $d/\lambda=1.0$, h/d=10, TM pol., $\phi=30°$, c/d=0.5, $\varepsilon^+=1$, $\varepsilon^-=2.5$	
	MM Li,[21] 50 layers, 41 modes	IM Li[21]	IM Goray, N=1500, P=750	CWM Mohar. *et al*,[22] 100 lay., 12 har., TE	IM Goray, N=1500, P=750		CM Plumey *et al*,[20] 131 har.	CWM Plumey *et al*,[20] 100 lay., 111 har.	IM Goray N=1500, P=750	MM Li,[25] 200 modes	IM Goray, N=1700, P=850
					TE pol.	TM pol.					
R_{-3}	–	–	–	–	–	–	–	–	–	–	–
R_{-2}	0.173	0.145	0.186	–	–	–	2.70	2.68	2.56	–	–
R_{-1}	0.0667	0.0816	0.0638	~1.0	1.31	0.541	0.1	0.096	0.102	0.150	0.330
R_0	0.0187	0.0306	0.0222	~0.5	0.590	0.288	0.006	0.006	0.0058	3.071	3.213
R_{+1}	–	–	–	–	–	–	–	–	–	–	–
R_{+2}	–	–	–	–	–	–	–	–	–	–	–
R_{+3}	–	–	–	–	–	–	–	–	–	–	–
T_{-3}	1.28	1.22	1.23	–	–	–	–	–	–	–	–
T_{-2}	21.3	21.2	21.2	~0.5	0.415	11.2	12.19	12.09	12.521	0.0709	0.0748
T_{-1}	46.2	46.4	46.3	51.0	51.5	43.4	21.99	22.01	22.08	13.89	13.12
T_0	18.4	18.6	18.5	44.5	44.6	33.4	62.48	62.58	62.09	80.41	79.65
T_{+1}	12.6	12.7	12.4	2.5	2.15	11.6	0.532	0.536	0.451	2.40	2.45
T_{+2}	–	–	–	–	–	–	–	–	–	–	–
T_{+3}	–	–	–	–	–	–	–	–	–	–	–
Balan.	100.	100.38	99.92	100.	100.60	100.41	100.	100.	99.81	100.	98.84

In work[21] the conclusion has been made, that for such deep gratings the number of partition layers is not big enough as real calculated profile differs considerably from perfect sinusoidal profile. The result of the comparison for sinusoidal grating, given in Table 2, confirms this conclusion. For comparison, in this work the profile has been approximated with 500-2000 points to obtain accurate results for very deep gratings. Therefore, there are certain differences in the results given in the tables for the coupled-wave method, modal method and Chandezon method, and various variants of integral method. Out of the calculations performed by different methods with about the same accuracy, the calculation results obtained by integral method for non-lamellar profile types are preferable.

Table 2. TM Diffraction efficiencies of deep metallic gratings, %.

Order	Lamellar, $d/\lambda=1.0$, TM pol., $h/d=1$, $\phi=30°$, $\varepsilon^+=1$, $\varepsilon^-=(0.22+i6.71)^2$			Sinusoidal, $d/\lambda=1.7$, $h/d=1$, TM pol., $\phi=30°$, $\varepsilon^+=1$, $\varepsilon^-=(0.3+i7.0)^2$			Triangle, $\lambda/d=0.7$, TM pol., $h/d=1.0$, $\theta_2=90°$, $\phi=25°$, $\varepsilon^+=1$ $\varepsilon^-=-21+i.60.4$			Triangle, $\lambda/d=0.5$, $\theta_1=30°$, $\theta_2=60°$, $\phi=15°$, $\varepsilon^+=1$, TM, $\varepsilon^-=(1.0+i5.0)^2$	
	MM Li,[23] 121 modes	CWM Granet *et al*,[26] 121 har.	IM Goray, N=500, P=250	MM Li,[21] 105 modes	IM Li[21]	IM Goray, N=500, P=250	CM Plumey *et al*,[20] 131 har.	CWM Plumey *et al*,[20] 100 lay., 111 har.	IM Goray, N=500, P=500	CM Li *et al*,[27] 51 har.	IM Goray, N=500, P=250
R_{-2}	–	–	–	12.64	15.7	18.81	46.88	42.75	46.39	70.04	69.80
R_{-1}	10.16	10.15	10.16	6.03	7.9	10.96	10.39	10.43	10.64	2.767	2.866
R_0	84.84	84.74	84.32	66.09	56.6	57.89	1.697	1.459	1.595	2.499	2.566
R_{+1}	–	–	–	–	–	–	–	–	–	0.9757	1.063
Absorp.	5.0	5.11	4.99	15.24	–	12.55	41.03	45.37	41.89	23.72	23.78
Balance	100.	100.	99.47	100.	–	100.22	100.	100.	100.52	100.	100.07

Table 3. TM diffraction efficiencies of very deep and high conducting metallic gratings, %.

Order	Sine, $d/\lambda=1.7$, $h/d=2$, TM pol., $\phi=30°$, $\varepsilon^+=1$, $\varepsilon^-=(0.3+i7.0)^2$		Triangle, $d/\lambda=10.0$, $h/d=2$, TM polarization, $\theta_1=90°$, $\phi=-3°$, $\varepsilon^+=1$, $\varepsilon^-=(6.43+i39.8)^2$			Lamellar, $d/\lambda=1.0$, TM pol., $h/d=4.8$, $\phi=30°$, $\varepsilon^+=1$, $\varepsilon^-=(0.22+i.6.71)^2$		Lamellar., $d/\lambda=1.0$, $h/d=1$, TM polarization, $\phi=30°$, $\varepsilon^+=1$, $\varepsilon^-=(11.5+i.67.5)^2$		
	CM Li,[25] 41 harm.	IM Goray, N=1700, P=850	CM Li,[25] 451 harm.	IM i.c. Goray, N=2000, P=1000	IM Goray, N=1000, P=100	CWM Granet *et al*,[26] 121 harm.	IM Goray, N=1800, P=900	MM Li,[25] 400 modes	IM i.c, Goray, N=1000, P=500	IM Goray N=1800, P=900
R_{-6}	–	–		0.644	0.736	–	–	–	–	–
R_{-5}	–	–	1.073	1.714	1.265	–	–	–	–	–
R_{-4}	–	–	2.229	2.161	2.352	–	–	–	–	–
R_{-3}	–	–	32.47	31.28	32.12	–	–	–	–	–
R_{-2}	42.21	41.39	6.974	12.39	8.455	4.99	8.116	95.55	97.92	93.78
R_{-1}	14.44	13.69	1.089	3.197	1.202	49.95	44.27	0.0522	0.0053	0.0461
R_0	24.80	24.55	0.0342	0.0510	0.0727	–	–	–	–	–
R_1	–	–	0.356	0.477	0.441	–	–	–	–	–
R_2	–	–	0.960	1.113	1.013	–	–	–	–	–
R_3	–	–	20.15	21.53	18.34	–	–	–	–	–
R_4	–	–	12.35	14.05	11.10	–	–	–	–	–
Absorp.	18.56	18.46	13.12	1.57	13.72	54.06	46.15	4.40	1.12	4.44
Balance	100.	98.09	100.	99.95	99.44	100.	98.54	100.	99.04	98.27

The examples of TM efficiency calculation are given in Tables 2-3 for deep and very deep reflecting gratings with various profiles of a groove and refractive index of metal, including for middle IR range. It is known, that efficiency calculations for finite-conductive metallic gratings in near and middle IR ranges for TM polarization are difficult for many methods, including the integral method, because of high refractive indices of grating materials. For such examples the calculations for aluminum grating with asymmetrical triangular profile (with a vertical left facet) for $\lambda/d = 0.1$, $h/d = 2$, and $\lambda = 4$ µm were included in study at an incident angle of 3 degree with respect to the less abrupt facet (see column 2 in Table 3), and, also, for golden lamellar grating (see column 4 in Table 3) for $\lambda/d = h/d = 1$ and $\lambda = 10$ µm with parameters from.[23] The method offered in[23] for wavelength of 10 µm and TM polarization has bad convergence:[24] the value of absorption for this point from[23] is more than 10%, whereas other predictions made with the help of integral and modal[25] methods give a value of about 4-5%%. For these points the results obtained by integral method within approximation of infinite conductivity and multiplied by Fresnel reflection factor also are given. From comparison one can conclude, that approximation of perfect conductivity, contrary to the existing opinion,[1,2] for such deep gratings for 4 µm and even for 10 µm does not give correct results for TM polarization. It is evident from value of absorption, which has been accurately calculated by the presented integral method. As for the essential difference in results from column 2 in Table 3, it is, probably, due to slow convergence of Chandezon method for this point because of the small wavelength-to-period ratio. The results from column 3 in Table 3 calculated with the help of our program are not so good in comparison with results,[26] due to slow convergence of the modified integral method for such a deep grating. However, there is no doubt they converge to values close to values from.[26]

As one can see from Tables 1-3, the efficiencies obtained by other rigorous methods and authors, agree well, despite of the very large depth, high conductivity and TM polarization, with values given in this work, especially, for the highly effective orders. This coincidence is especially impressing for profiles of a groove having vertical slopes considered to be the most "difficult" cases for an integral method. Almost for all results, obtained by the author, the total error for energy balance did not exceed 1%. For the depths about one period it has value that is several times or an order of magnitude less.

Our experience in numerical calculations proves, that for high enough values of N the modified integral method gives stable and equally good TE/TM convergence for deep and very deep dielectric and metallic gratings for, practically, any parameters and any form of a groove profile, including real, i.e. measured by any method. At that, optimization of parameter P is necessary seldom, though the time of calculation with the above-stated accuracy of one point for such deep diffraction gratings makes up from several seconds till several hours on mentioned PC. In practice, it is a rare case to investigate very deep gratings and, as a rule, there is no necessity for calculations with very high accuracy. For example, from energy balance it is sufficient to have only 150 points to obtain a total error no more than 1% for calculation of the grating from the data of column 1 in Table 1, i.e. 10 times less, than it is required for the result in the table. At that, the time of calculation in accordance with (3.8) decreases, approximately, 1000 times, and the relative error for the most and least accurate results makes up from several percents for high efficiency orders up to several tens percents for low efficiency orders. Hence, for N = 150 the accuracy is good enough for correct prediction of high efficiency values and insufficient - for low ones.

7. CONCLUSION

In conclusion it would be desirable to compare resources of the developed modified integral method relative to other known realizations of methods (coupled-wave, modal and Chandezon) for calculations for deep and very deep gratings, including those with a real profile of grooves.

The coupled-wave and modal methods are certainly preferable for calculations of gratings with lamellar profile, as, in this case, convergence and accuracy of these methods depend slightly on grating depth.[21-24] For other types of perfect profiles, these methods and Chandezon method are comparable in accuracy and computing time with the integral one. The coupled-wave and modal methods require not less than 50-100 layers of partition for accurate approximation of gratings with $h/d = 10$ and $d/\lambda = 1$.[21-26] In the case of the high ratios d/λ this number must proportionally be increased, especially, for TM polarization. In the case of metals, the internal convergence of methods themselves is deteriorating with increase of d/λ and conductivity of material. This requires of increase of truncation parameter, on which the computing time depends cubically.[24] All this results in long time of efficiency calculation for deep and very deep non-lamellar gratings, despite of certain simplicity and fast convergence of the successful implementation of these methods for lamellar profile. At last, these methods are considered to be practically unacceptable for gratings with real, i.e. measured profiles of a groove. The profiles, measured by any modern method, contain, as a rule, more than 100 points[17-19] (even 500 and more). For the accurate approximation of such profiles it is required some times even more partition layers, i.e. it is necessary to use about several hundredths, and even thousands of partition layers. Besides, during such calculations it is necessary to use increased accuracy of the solution for each layer, as the total error increases with growth of number of layers. Therefore, the accurate efficiency calculations for deep gratings with the real form of grooves performed by modal or coupled-wave methods on modern PC, even for individual points, are considered by the author rather problematic. This seems to be true for Chandezon method as well, that weakly converges at calculations for large d/λ (especially, for the high orders) and at sharp jumps of groove profile function derivative, what is typical for real profiles.

Unfortunately, examples of efficiency calculations for many types of gratings: echelle;[3,8,18,25] for soft x-ray and XUV ranges,[3,7,12,13,15] including with the real groove profile;[4,5,8,17] with a real profile for other spectral ranges;[8,19] have not been included in this work. All these examples can be found in the cited above literature or in the special future investigations.

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