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Energy-absorption calculus for multi-boundary conical-diffraction gratings

Leonid I. Goray

St. Petersburg Academic University – Nanotechnology Research and Education Center of the Russian Academy of Sciences (RAS), Russia;
Institute for Analytical Instrumentation, RAS, Russia; e-mail: lig@pcgrate.com

The author presents a general formula derived from the earlier developed boundary integral equation theory, which is important for absorption calculations of multi-boundary gratings in conical diffraction. Examples of absorption computations of a photonic crystal supporting polariton-plasmon excitation and an x-ray-grazing-incidence multilayer grating are considered. The formula tested has been found universal and accurate for analyzing various in-plane and off-plane diffraction grating problems.

1 Introduction

The boundary integral equation method is presently universally recognized as one of the most developed and flexible approaches to accurate numerical solution of diffraction grating problems. Viewed in the historical context, this method was the first to offer a solution to vector problems of light diffraction by optical gratings with a high enough accuracy and to demonstrate remarkable agreement with experimental data. In many cases it offers the only possible way to followup in research. This should be attributed to the high accuracy and good convergence of the method, especially for the TM polarization plane.

The electromagnetic formulation of conical diffraction by gratings reduces Maxwell equations to a system of two Helmholtz equations in $\mathbb{R}^2$, which are coupled by transmission conditions at interfaces between different materials and a subject to radiation conditions in the upper and lower mediums. The integral equations obtained using boundary integrals of the single and double layer potentials including the tangential derivative of single layer potentials interpreted as singular integrals can be found elsewhere [1]. In the case of classical diffraction, when the incident wave vector is orthogonal to the groove (z-) direction, the system degenerates to independent transmission problems for the two basic polarizations of the incident wave, whereas for the case of conical diffraction (Fig. 1) the boundary values of the z-components as well as their normal and tangential derivatives at the interface are coupled. The boundary profiles of the layers can be separated, i.e., the maximal y value of a given profile is strictly less than the minimal y value of the next profile above (Fig. 2) or, vise versa, penetrating (Fig. 3).

One of the most important accuracy criteria based on a single computation is the energy balance that can be generalized in the lossy case. In this paper we provide an important formula for the direct calculation of the absorption of multi-boundary gratings in general conical mounts. Besides, a couple of numerical examples of absorption calculus are presented for well known optical applications of gratings. More specifically, they are: anomalously absorbing photonic band gaps (PBGs) with metallic nanorods illuminated at normal incidence in the visible-infrared range and blazed multilayer gratings working in grazing conical diffraction in the x-ray range.

2 Diffraction problem

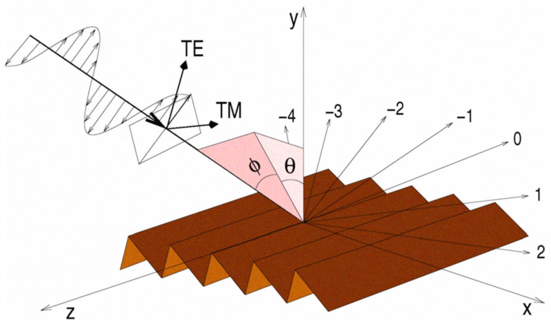

Figure 1: Schematic conical diffraction by a grating.

In the multi-boundary diffraction problem one has to deal with cylindrical surfaces $\Sigma_n \times \mathbb{R}$, $n = 0, ..., N-1$, either open or closed, which are d-periodic in x and whose generatrices are parallel to the z-axis (Fig. 2). The surfaces separate $N+1$

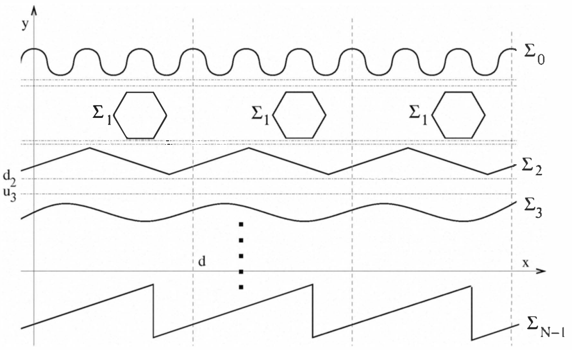

Figure 2: Schematic cross section of a grating with separated boundaries.

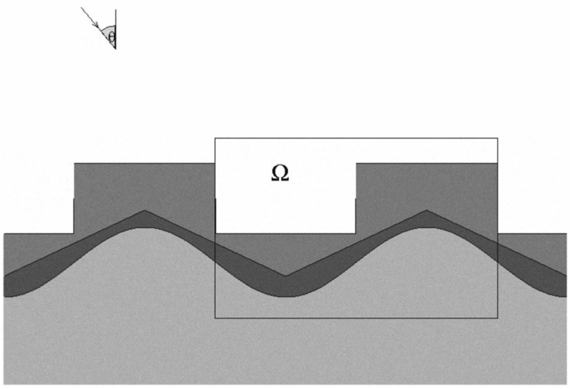

Figure 3: Schematic cross section of a grating with penetrating boundaries.

periodic regions $G_n \times \mathbb{R}$, filled with material of constant permittivity and permeability. The grating structure is characterized by piecewise constant functions of electric permittivity ε and magnetic permeability μ, which are d-periodic in x, homogeneous in z, and have jumps at the surfaces Σ_n. The values of these functions in the semi-infinite regions $G_0 \times \mathbb{R}$ above and $G_N \times \mathbb{R}$ below the inhomogeneous structure are denoted by ε_0, μ_0 and ε_N, μ_N, respectively. We assume that $\lambda = 2\pi c/\omega$ with a light velocity c at a given pulsatance ω and the incident time-harmonic field with polarization vectors $\mathbf{p}$ and $\mathbf{s}$ defined later is given by

$$(\mathbf{E}^i, \mathbf{H}^i) = (\mathbf{p}, \mathbf{s})\, \mathrm{e}^{-\mathrm{i}\omega t}\, \mathrm{e}^{\mathrm{i}(\alpha x - \beta y + \gamma z)},$$

$(\alpha, -\beta, \gamma) = \omega\sqrt{\varepsilon_0\mu_0}(\sin\theta\cos\phi, -\cos\theta\cos\phi, \sin\phi)$, and $|\theta|, |\phi| < \pi/2$.

Due to the periodicity of the surfaces the incident wave is scattered into a finite number of plane waves in $G_0 \times \mathbb{R}$ and also in $G_N \times \mathbb{R}$ if $\varepsilon_N\mu_N > 0$. The wave vectors of these outgoing orders lie on the surface of a cone whose axis is parallel to the z-axis. Therefore one speaks of conical diffraction. Classical diffraction corresponds to $\gamma = 0$, whereas $\gamma \neq 0$ characterizes conical diffraction. Using the representation of the total field $\mathbf{E}(x, y, z) = E(x, y)\, \mathrm{e}^{\mathrm{i}\gamma z}$, $\mathbf{H}(x, y, z) = \sqrt{\varepsilon_0/\mu_0}B(x, y)\, \mathrm{e}^{\mathrm{i}\gamma z}$ the system of time-harmonic Maxwell equations transforms to 2D Helmholtz equations in the domains G_n, where ε and μ are constant,

$$(\Delta + (\omega\kappa)^2)E(x, y) = (\Delta + (\omega\kappa)^2)B(x, y) = 0 \quad (1)$$

with the coefficient function $(\omega\kappa)^2 = \omega^2\varepsilon\mu - \gamma^2$ piecewise constant and d-periodic in x.

It can be shown that under the condition $\kappa \neq 0$, which will be assumed throughout, the z-components E_z, B_z of the vector functions E and B determine the total electromagnetic field $(\mathbf{E}, \mathbf{H})$. The continuity of the tangential components of $\mathbf{E}$ and $\mathbf{H}$ on the surface Σ_n implies jump conditions for E_z, B_z in the form

$$\begin{aligned} \big[E_z\big]_{\Sigma_n} &= \big[H_z\big]_{\Sigma_n} = 0, \\ \Big[\frac{\varepsilon\, \partial_\nu E_z}{\kappa^2}\Big]_{\Sigma_n} &= -\varepsilon_0 \sin\phi \Big[\frac{\partial_t B_z}{\kappa^2}\Big]_{\Sigma_n}, \\ \Big[\frac{\mu\, \partial_\nu B_z}{\kappa^2}\Big]_{\Sigma_n} &= \mu_0 \sin\phi \Big[\frac{\partial_t E_z}{\kappa^2}\Big]_{\Sigma_n}, \end{aligned} \quad (2)$$

where $[\,.\,]$ denotes the jump of functions on Σ_n, and $\partial_\nu = \nu_x\partial_x + \nu_y\partial_y$ and $\partial_t = -\nu_y\partial_x + \nu_x\partial_y$ are the normal and tangential derivatives on Σ_n, respectively. The z-components of the incoming field

$$E_z^i(x, y) = p_z\, \mathrm{e}^{\mathrm{i}(\alpha x - \beta y)},$$
$$B_z^i(x, y) = s_z\, \mathrm{e}^{\mathrm{i}(\alpha x - \beta y)}\sqrt{\mu_0/\varepsilon_0} = q_z\, \mathrm{e}^{\mathrm{i}(\alpha x - \beta y)}$$

are α-quasiperiodic in x of period d. Here the vector $\mathbf{s}$ is orthogonal to the plane spanned by $\mathbf{k}$ and the grating normal $\nu = (0, 1, 0)$ and $\mathbf{p}$ lies in that plane:

$$\mathbf{s} = \mathbf{k} \times (0, 1, 0)/|\mathbf{k} \times (0, 1, 0)|, \ \ \mathbf{p} = \mathbf{s} \times \mathbf{k}/|\mathbf{k}|.$$

If $\mathbf{k} = (0, -k, 0)$, we set $\mathbf{s} = (0, 0, 1)$ and hence $\mathbf{p} = (1, 0, 0)$. Then, the incident plane wave is given by its polarization angles

$$\delta = \arctan[|(\mathbf{E}^i, \mathbf{s})|/|(\mathbf{E}^i, \mathbf{p})|],$$
$$\psi = -\arg[(\mathbf{E}^i, \mathbf{s})/(\mathbf{E}^i, \mathbf{p})],$$

where $\delta \in [0, \pi/2]$, $\psi \in (-\pi, \pi]$.

We seek a bounded H^1-regular solution (E_z, B_z) which is α-quasi-periodic in x $(u(x + d), y) =$

$e^{i\alpha d}\,u(x,y))$ and satisfies the radiation conditions

$$(E_z,B_z)=(E_z^i,B_z^i)+\sum_{m\in\mathbb{Z}}(E_0^m,B_0^m)\,e^{i(\alpha_m x+\beta_0^m y)}$$
$$\text{for } y\ge \sup\Sigma_0,$$
$$(E_z,B_z)=\sum_{m\in\mathbb{Z}}(E_N^m,B_N^m)\,e^{i(\alpha_m x-\beta_N^m y)}$$
$$\text{for } y\le \inf\Sigma_{N-1}, \qquad (3)$$

$\alpha_m=\alpha+2\pi m/d$, $\beta_n^m=\sqrt{\omega^2\varepsilon_n\mu_n-\gamma^2-\alpha_m^2}$ with $0\le\arg\beta_n^m<\pi$. In the following it is always assumed that besides $\varepsilon_0,\mu_0>0$

$$0\le\arg\varepsilon,\arg\mu\le\pi,\arg(\varepsilon\mu)<2\pi\,,$$

which holds for all existing optical (meta)materials [4]. Then the electromagnetic formulation of conical diffraction on multi-boundary gratings is equivalent to (1)–(3) for (E_z,B_z).

To solve the multi-boundary integral equations we use the effective recursive algorithms [2, 3]. For profiles which are separated by horizontal lines (Fig. 2) or penetrating (Fig. 3) we use the Separating or Penetrating solvers, respectively, i.e. a consecutive solution of one-profile problems. The choice of a numerical method to solve the multi-boundary integral equations is such that not even necessary to use the same method for every boundary provided that adjacent boundary solvers have a common data interface. The equivalence of the system to the differential formulation of conical diffraction has been shown in [4]. Moreover, the existence and uniqueness of solutions (Fredholm property of respective operators) in appropriate function spaces ensure the convergence of numerical methods.

3 Energy conservation criteria

Diffraction efficiencies or far field patterns for the reflected and transmitted fields can easily be found from the corresponding boundary values. The efficiency of a diffracted order represents the proportion of power radiated in each order. Defining the power as the flux of the Pointing vector modulus $|\mathbf{S}^{\mathrm{inc}}|=\mathrm{Re}\,(\mathbf{E}^i\times\overline{\mathbf{H}^i})/2$ ($\overline{X}$ denotes the complex conjugate of X) through a normalized rectangle parallel to the (x,z)-plane, the ratio of the power of reflected or transmitted propagating orders and of the incident wave gives the sum of diffraction efficiencies of reflected orders

$$R=\sum_{\beta_0^m>0}\frac{\beta_0^m}{\beta}\big(|E_0^m|^2+|B_0^m|^2\big)$$

or transmitted orders

$$T=\sum_{\beta_N^m>0}\frac{\beta_N^m}{\beta}\Big(\frac{\varepsilon_N}{\varepsilon_0}|E_N^m|^2+\frac{\mu_N}{\mu_0}|B_N^m|^2\Big)\,.$$

If the multi-boundary grating is perfectly conducting, $\mathrm{Im}\,\nu_N=\infty$, and there is no any energy absorption in the grating layers, $\mathrm{Im}\,\nu_j=0$, $j=1,\dots,N-1$, then the energy conservation law is expressed by the standard energy criterion under unitary normalization conditions

$$R=1.$$

If the grating is lossless, $\mathrm{Im}\,\nu_j=0$, $j=0,\dots,N$, then the energy conservation law is expressed by a similar energy criterion

$$R+T=1.$$

If $\mathrm{Im}\,\nu_j>0$ for any $j=1,\dots,N$, then there is some energy absorption in grating layers or/and in the substrate. Thus the usual law of the energy conservation, the sum of efficiencies of all reflected and transmitted orders should be equal to the power of the incident wave, does not hold. In a general case,

$$A+R+T=1, \qquad (4)$$

where A is called the absorption coefficient or simply the absorption in the given diffraction problem. This requirement is a convenient single computation tool to check the quality of the numerical solution [3]. Besides being physically meaningful, expression (4) is very useful as one of numerical accuracy tests for computational codes and especially important for x-ray–EUV gratings, photonic crystals, metamaterials, and perfect absorbers where absorption plays a predominant role. In the lossy case, one needs an independently calculated quantity A to verify Eq. (4). For such a quantity, we use the absorption integrals derived below.

4 Energy absorption integrals

Because of the problem being invariant under translation by an integer number of periods along the axis perpendicular to the grooves, one may restrict oneself to an analysis of the heat power loss A per grating period. A can be calculated as a difference between the energy fluxes that have crossed the upper, Γ_0 (Γ_n denotes one period of Σ_n), and the lower, Γ_{N-1}, boundaries of the multilayer structure through a periodic cell Ω bounded by the $x=0$,

$x = d$, $z = 0$, $z = 1$, and $y = \pm D/2$ planes, which contains Γ_0 and Γ_{N-1} (Fig. 3):

$$A = \int_0^1 dz \int_{\Gamma_0} \mathbf{S}_0^- \mathbf{n}_0 ds - \int_0^1 dz \int_{\Gamma_{N-1}} \mathbf{S}_{N-1}^- \mathbf{n}_{N-1} ds, \quad (5)$$

where $\mathbf{S}_0^-$ and $\mathbf{S}_{N-1}^-$ are time-averaged complex Poynting vectors calculated at the upper and lower boundaries, $\mathbf{n}_0$ and $\mathbf{n}_{N-1}$ are unit vectors of the normal, which are interior to the regions under study, and arc length integration is performed along the cut of the boundaries by the $z = 0$ plane.

The expression of the conservation of energy can be derived from a variational equality for E_z and B_z in Ω. Suppose that E_z, B_z are a solution of the partial differential formulation of conical diffraction, Eqs. (1), (2), and (3), we multiply Eqs. (1) respectively with

$$\frac{\varepsilon}{\varepsilon_0 \kappa^2}\overline{E_z} \quad \text{and} \quad \frac{\mu}{\mu_0 \kappa^2}\overline{B_z},$$

and apply the second Green's formula in the subdomains $\Omega \cap G_{0,N}$. Then by using the quasiperiodicity of E_z, B_z, jump relations (2), and outgoing wave conditions (3) one derives the expression for the absorption $A_{\Gamma_{n-1}}$ under any boundary Γ_{n-1} [1]

$$A_{\Gamma_{n-1}} = \frac{1}{\beta}\,\mathrm{Im}\left(\frac{\kappa_{n-1}^2}{\kappa_n^2}\Big(\frac{\varepsilon_n}{\varepsilon_{n-1}}\int_{\Gamma_{n-1}} \partial_n E_z \overline{E_z} + \frac{\mu_n}{\mu_{n-1}}\int_{\Gamma_{n-1}} \partial_n B_z \overline{B_z} + 2\sin\phi\,\mathrm{Re}\int_{\Gamma_{n-1}} E_z \partial_t \overline{B_z}\Big)\right). \quad (6)$$

Note that ε_{n-1} and μ_{n-1} are positive, and $\mathrm{Im}\,\varepsilon_n \neq 0$ or $\mathrm{Im}\,\mu_n \neq 0$. Taking into account (5) and (6) we obtain the energy absorption formula for absorbing multi-boundary gratings in conical diffraction:

$$A = \frac{1}{\beta}\,\mathrm{Im}\left(\frac{\kappa_0^2}{\kappa_1^2}\Big(\frac{\varepsilon_1}{\varepsilon_0}\int_{\Gamma_0} \partial_n E_z \overline{E_z} + \frac{\mu_1}{\mu_0}\int_{\Gamma_0} \partial_n B_z \overline{B_z} + 2\sin\phi\,\mathrm{Re}\int_{\Gamma_0} E_z \partial_t \overline{B_z}\Big)\right) - \frac{1}{\beta}\,\mathrm{Im}\left(\frac{\kappa_0^2}{\kappa_N^2}\Big(\frac{\varepsilon_N}{\varepsilon_0}\int_{\Gamma_{N-1}} \partial_n E_z \overline{E_z} + \frac{\mu_N}{\mu_0}\int_{\Gamma_{N-1}} \partial_n B_z \overline{B_z} + 2\sin\phi\,\mathrm{Re}\int_{\Gamma_{N-1}} E_z \partial_t \overline{B_z}\Big)\right). \quad (7)$$

In the case $\phi = 0$ this formula provides the expression of the heat absorption energy for in-plane (classical) diffraction derived in [5]. In terms of the solution w, τ of the integral equations [1] the absorption energy (7) can be given by the boundary single-layer potentials V_n^-, double-layer potentials L_n^-, singular operators J_n^- of tangential derivatives of single-layer potentials, and the unitary operator I

$$A = \frac{1}{\beta}\,\mathrm{Im}\left(\frac{\kappa_0^2}{\kappa_1^2}\int_{\Gamma_0}\Big(\frac{\varepsilon_1}{\varepsilon_0}(L_0^- - I)w\overline{V_0^- w} + \frac{\mu_1}{\mu_0}(L_0^- - I)\tau\overline{V_0^-\tau}\Big)\right) + \frac{2\sin\phi}{\beta}\,\mathrm{Im}\,\frac{\kappa_0^2}{\kappa_1^2}\,\mathrm{Re}\int_{\Gamma_0} V_0^- w \overline{J_0^-\tau} - \frac{1}{\beta}\,\mathrm{Im}\left(\frac{\kappa_0^2}{\kappa_N^2}\int_{\Gamma_{N-1}}\Big(\frac{\varepsilon_N}{\varepsilon_0}(L_{N-1}^- - I)w\overline{V_{N-1}^- w} + \frac{\mu_N}{\mu_0}(L_{N-1}^- - I)\tau\overline{V_{N-1}^-\tau}\Big)\right) - \frac{2\sin\phi}{\beta}\,\mathrm{Im}\,\frac{\kappa_0^2}{\kappa_N^2}\,\mathrm{Re}\int_{\Gamma_{N-1}} V_{N-1}^- w \overline{J_{N-1}^-\tau}. \quad (8)$$

5 Examples of absorption calculus

The numerical implementation approach expedient for the calculation of far-fields and polarization properties of conical diffraction by gratings was described in Refs. [1, 2, 6]. Here we present a few numerical experiments taken from important applications of absorption gratings. The presented results demonstrate the impact of absorption on diffraction in PBGs and x-ray multilayer gratings.

5.1 PBG with Au rectangular nanorods

In this Subsection, we are going to analyze numerically the absorption of photonic crystal slabs supporting polariton-plasmon excitation with nanowires invariant with respect to the z axis. Though surface plasmon exitation plays a predominant part in metallic PBGs, other types of electromagnetic resonances can also exist in complex material structures: Rayleigh anomalies, Fabry–Perot and Bragg resonances, waveguiding anomalies, etc. The vital role of the absorption of PBGs and metamaterials in the visible and near infrared regions is well known. In conical diffraction the influence of possible types of waves can be mixed [2].

The grating model contains closed boundaries (inclusions) of a simple cross section embedded in a homogeneous medium with dielectric permittivity ε_1 and magnetic susceptibility μ_1. We are going to deal here only with materials with $\mu_n = 1$, although the model is applicable to other cases as well, including metamaterials [2]. The dependence of the dielectric permittivity ε_2 of the material of nanorods on the incident photon frequency is assumed to be known. The lower medium and the upper one are likewise assigned pairs of material constants, but one may conceive of more complicated cases of multilayer structures as well. The model allows also arbitrary incidence of, in the general case, elliptically polarized radiation on PBGs, which is prescribed by two angles of incidence and two angles of polarization.

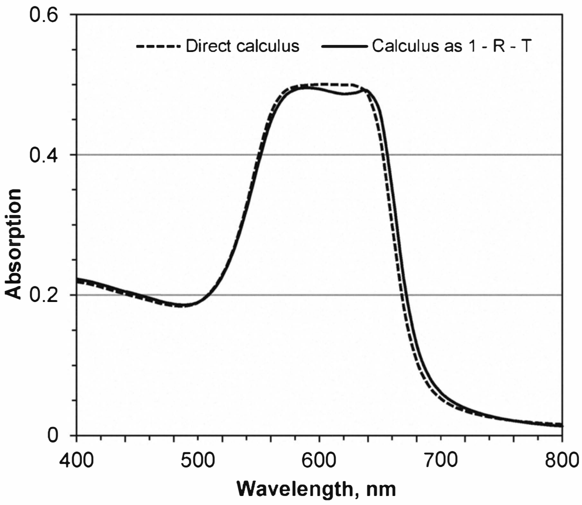

Figure 4: Absorption of a grating with Au rectangular nanorods embedded in a dielectric medium vs wavelength.

Figure 4 displays for comparison theoretical spectra of energy absorbed by a PBG with Au nanowires of the rectangular cross section of the area of 15×50 nm^2 studied in the 400–800-nm range (visible and near-infrared). In this example we consider the TM-polarized light (the plane of polarization is perpendicular to the lines) normally falling on Au nanowires with $d = 200$ nm embedded in a dielectric matrix with $\varepsilon_1 = 2.25$ and refractive indices of Au taken from [7]. The orientation of the rods is chosen in such a way that light normally falls on a long side of a rod. The absorption spectra of the PBG were calculated by two different boundary integral equation codes based on the Separating solvers [2, 6]: (i) using direct calculations of absorption integrals by Eq. (7) and (ii) using the usual indirect approach by Eq. (4). For the method (i) we use the electromagnetic field calculated by Raleigh expansions similar to those of Eqs. (3). It is worth note, the number of accounting propagating and evanescent orders, which are computed with desired accuracy, should be enough. The rule to find this number while is not clear mathematically, so it should be optimized numerically. For this example we take into account one propagating and four evanescent orders. As seen from Fig. 4, absorption spectra exhibit a small difference, about a few percent, in the vicinity of and, particularly, around the plasmon-polariton anomaly. Thus, examining the two curves, we see a good agreement, which evidences applicability of both numerical approaches to analysis of absorption of such PBGs.

A small number of collocation points ($\mathcal{N} = 100$) were used to compute these examples which allocate $\sim$ 0.5 MB of RAM. The relative error calculated from the energy balance using the absorption integrals of Eq. (7) is $\sim 10^{-3}$. The average time taken up by one point on a portable workstation IBM® ThinkPad® R50p with an Intel® Pentium® M 1.7 GHz processor and 2 GB of RAM is $\sim$ 1 sec when operating on Windows® XP Pro.

5.2 X-ray multilayer grating

Multilayer coated blazed gratings with high groove density are the best candidates for use in high resolution EUV and x-ray spectroscopy. Theoretical and experimental analysis show that such a grating can be potentially optimized for high dispersion and spectral resolution in a desired high diffraction order without significant loss of diffraction efficiency. In order to realize this potential, the grating should have a perfect triangular groove profile and its absorption should be minimized [8]. The grazing-incidence conical-diffraction mounting in which the direction of incident light is confined to a plane parallel to the direction of the grooves has the unique property of maintaining high and sustained diffraction efficiency due to an additional angular parameter. In this Subsection, we analyze the optical absorption of a blazed multilayer grating working in grazing conical diffraction in the soft x-ray range.

In Fig. 5 the absorption of the 10000 /mm blazed Si grating coated with 60 bi-layers of W/B_4C is calculated for the TE polarized ($\delta = 90°$) incidence radiation with $\lambda = 1.3$ nm and $\theta = 6°$ as a function of the azimuthal angle. The grating has a triangular groove profile with the blaze angle of 6° and antiblaze angle of 64.53° and a conformal multilayer coating with the thicknesses of W and B_4C layers,

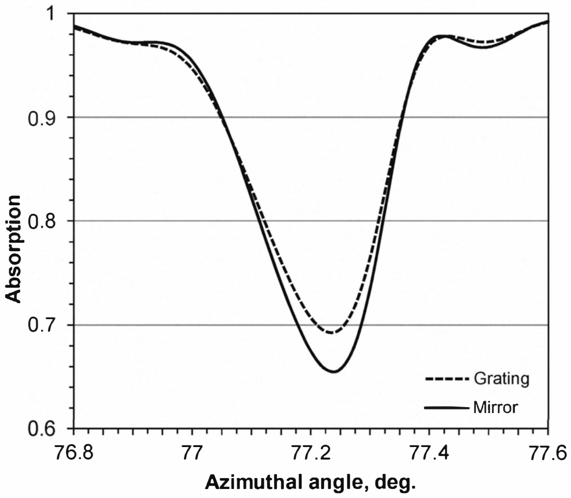

Figure 5: Absorption of W/B_4C multilayer structures working in a conical mount vs incidence angle of x-ray radiation.

0.6006 nm and 2.4024 nm, respectively. The refractive indices of Si, W, and B_4C were taken from [9]. Figure 5 displays for comparison theoretical absorption spectra of a Si mirror coated with the same multilayer and working in the same mount. As one can see in Fig. 5, for the defined polar angle the grating and mirror absorptions are close in the azimuthal angle range investigated. The grating absorption minima less than 70% can be obtained for the azimuthal angle of $\sim 77.2°$. Thus, almost the all reflected energy can be directed into diffraction orders without additional losses for the grating absorption.

Only $\mathcal{N} = 400$ were used to compute this grating example which allocates $\sim$ 60 MB of RAM. The relative error calculated from the energy balance using Eq. (7) is $\sim 10^{-4}$. The average time taken up by one point on the same laptop is $\sim$ 1.5 hour when operating on Linux (kernel 2.6.17).

6 Conclusion

The author presents the expressions derived from the developed boundary integral equation theory, which are important for calculations of the absorption of general multi-boundary gratings working in conical diffraction mounts. The boundary absorption integrals developed and tested has been found as an accurate and universal tool for calculations of the energy balance of various periodical structures having separated or penetrating boundaries. The results of absorption calculus of the PBG supporting polariton-plasmon excitation in the visible–near-infrared and x-ray-grazing-conical-diffraction multilayer grating have been demonstrated.

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References

[1] Goray L.I., Schmidt G., 2010, Solving conical diffraction grating problems with integral equations, *J. Opt. Soc. Am. A*, Vol. **27**, pp. 585–597.

[2] Goray L.I., Schmidt G., 2012, Analysis of two-dimensional photonic band gaps of any rod shape and conductivity using a conical-integral-equation method, *Phys. Rev. E*, Vol. **85**, pp. 036701-1–12.

[3] Goray L.I., Kuznetsov I.G., Sadov S.Yu., Content D.A., 2006, Multilayer resonant subwavelength gratings: effects of waveguide modes and real groove profiles, *J. Opt. Soc. Am. A*, Vol. **23**, pp. 155–165.

[4] Schmidt G., 2010, Boundary Integral Methods for Periodic Scattering Problems, in *Around the Research of Vladimir Maz'ya II. Partial Differential Equations, Springer*, pp. 337–364.

[5] Goray L.I., 2010, Application of the boundary integral equation method to very small wavelength-to-period diffraction problems, *Waves Random Media*, Vol. **20**, pp. 569–586.

[6] Goray L.I., 2009, Specular and diffuse scattering from random asperities of any profile using the rigorous method for x-rays and neutrons, *Proc. SPIE*, **7390**, pp. 73900V-1–11.

[7] Palik E.D., ed., 1985, Handbook of Optical Constant of Solids, *Academic, Orlando.*

[8] Voronov D.L., Goray L.I., Warwick T., Yashchuk V.V., Padmore H.A., 2012, Optimization of multilayer coated blazed gratings for soft x-ray applications, to be published in *J. Opt. Soc. Am. A.*

[9] `http://henke.lbl.gov/optical_constants/.`