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Numerical analysis of the efficiency of multilayer-coated gratings using integral method

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Abstract

An analysis is made of a rigorous and an approximate approach to the solution of the diffraction problem for a multilayer-coated X-ray grating by the integral equation formalism. Whereas a rigorous analysis involving the integral method requires a lot of computer resources, even for gratings with a small number of layers, the approximate approach based on a modification of the solution of the integral equation at the lower boundary with a finite conductivity is practically independent of the number of layers and is readily tractable with the use of a standard PC. The efficiencies of multilayer gratings measured at grazing angles with synchrotron soft X-ray radiation are compared with the values calculated using the integral approaches for ideal groove profiles.

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1. Introduction

Multilayer-coated diffraction gratings offer the best promise for use in the short-wavelength range from hard X-ray to EUV, but modeling of their efficiency by rigorous methods meets with difficulties not encountered in calculation of bulk gratings [1]. The scalar theory of diffraction or application of the perfect conductivity approximation cannot predict exact results; especially, for grazing incidence angles, in the TM polarization, and in high orders. One may refer, for instance, to a rigorous calculation based on the differential method, but performed only for the ideal sawtooth profile with a small number of layers and only in the TE polarization [2]. The IESMP integral method is

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capable of handling bulk gratings with real groove profiles measured by scanning probe microscopy or any other modern tool [3]. The integral method is also applied successfully to studies of the efficiencies of so called lamellar multilayer amplitude gratings (LAMGs), which are the kind of the Bragg optics [4].

The present paper reports on an integral method applied to multilayer-coated gratings and referred to in the literature as "modified" [5,6]. It was employed to advantage to carry out the first calculation of the accurate efficiency of X-ray gratings with near-normal incidence, either coated by several layers or multilayered, with any groove profile, including a realistic (AFM-measured) groove shape [7,8], and with due account taken of random roughness [9–11]. The modified integral method permits easy modeling the efficiency of X-ray-range bulk real groove profile gratings operating at grazing incidence [12]. Application of the exact method requires, however, considerable computational resources, even in the case of gratings with a small number of layers. For instance, computation of one point for an X-ray grating with several tens of layers takes up many hours of work on a modern PC.

This stimulated the present author to develop in Section 2 along with the rigorous method an approximate approach for calculating the efficiency of grazing-incidence multilayer gratings, which is based on a modification of the solution to the integral equation at the lower finite-conductivity boundary and does not depend on the number of grating layers. A criterion of obtaining accurate data provided by the approximation to the integral method for multilayer X-ray grating efficiency calculations is proposed, and the conditions of its application are analyzed in Section 3. Next, in Section 4 the rigorously calculated and measured efficiencies of multilayer gratings with an ideal groove profile are compared with approximate data. Finally, the conclusion is given in Section 5.

2. A rigorous and an approximate approaches to calculate the efficiency of a multilayer grating

The coupled integral equations for a multilayer grating made up of K boundaries, starting with the top one (first), can be cast using the second Green's identity and boundary conditions, similar to the way this is done for a grating with one interface separating two media [10]:

$$
\begin{aligned}
U_1(s_1)/2 = {} & U^i/2 + \int_{S_1} G_1^+(s_1, s_1')(c_j\, \mathrm{d}U_1(s_1')/\mathrm{d}n_1' \\
& - \mathrm{d}U^i(s_1')/\mathrm{d}n_1')\, \mathrm{d}s_1' \\
& + \int_{S_1} (\mathrm{d}G_1^+(s_1, s_1')/\mathrm{d}n_1')(U_1(s_1') \\
& - U^i(s_1'))\, \mathrm{d}s_1' \\
U_k(s_k)/2 = {} & \int_{S_k} c_j G_k^-(s_k, s_k')(\mathrm{d}U_k(s_k')/\mathrm{d}n_k')\, \mathrm{d}s_k' \\
& - \int_{S_k} (\mathrm{d}G_k^-(s_k, s_k')/\mathrm{d}n_k')\, U_k(s_k')\, \mathrm{d}s_k' \\
& + \int_{S_{k+1}} c_j G_{k+1}^+(s_k, s_{k+1}') \\
& \times (\mathrm{d}U_{k+1}(s_{k+1}')/\mathrm{d}n_{k+1}')\, \mathrm{d}s_{k+1}' \\
& + \int_{S_{k+1}} (\mathrm{d}G_{k+1}^+(s_k, s_{k+1}')/\mathrm{d}n_{k+1}') \\
& \times U_{k+1}(s_{k+1}')\, \mathrm{d}s_{k+1}' \\
U_{k+1}(s_{k+1})/2 = {} & \int_{S_{k+1}} c_j G_{k+1}^+(s_{k+1}, s_{k+1}') \\
& \times (\mathrm{d}U_{k+1}(s_{k+1}')/\mathrm{d}n_{k+1}')\, \mathrm{d}s_{k+1}' \\
& + \int_{S_{k+1}} (\mathrm{d}G_{k+1}^+(s_{k+1}, s_{k+1}')/\mathrm{d}n_{k+1}') \\
& \times U_{k+1}(s_{k+1}')\, \mathrm{d}s_{k+1}' - \int_{S_k} c_j G_k^-(s_{k+1}, s_k') \\
& \times (\mathrm{d}U_k(s_k')/\mathrm{d}n_k')\, \mathrm{d}s_k' \\
& - \int_{S_k} (\mathrm{d}G_k^-(s_{k+1}, s_k')/\mathrm{d}n_k')\, U_k(s_k')\, \mathrm{d}s_k', \\
U_K(s_K)/2 = {} & -\int_{S_K} c_j G_K^-(s_K, s_K') \\
& \times (\mathrm{d}U_K(s_K')/\mathrm{d}n_K')\, \mathrm{d}s_K' \\
& - \int_{S_K} (\mathrm{d}G_K^-(s_K, s_K')/\mathrm{d}n_K')\, U_K(s_K')\, \mathrm{d}s_K' \\
& k = 1, K-1;\, j = k-1, K
\end{aligned}
\tag{2.1}
$$

where s_k is the curvilinear coordinate of the boundary S_k, U^i is the incident field, U_k is the z-component of the electric or magnetic field at the kth boundary, $G_k{}^{\pm}$ is Green's function for the region above (+) or below (−) the kth boundary, $\boldsymbol{n}$ is the vector of the surface normal (directed from "−" to "+"), $c_j = 1$ for the TE polarization and

$c_j = \varepsilon_j$ for the TM polarization, and ε_j is the dielectric permittivity of the jth layer, starting from the top (zero) one.

Green's function and its normal derivative for the upper and lower regions separated by the kth boundary are calculated identically

$$\begin{aligned} G_k^{\pm}(x, y, s_k') &= \sum\nolimits_{n=-\infty}^{\infty}\{\exp[\mathrm{i}Kn(x - x_k'(s_k')) \\ &\quad + \mathrm{i}\beta_{k,n}^{\pm}|y - f_k(s_k')|]/\beta_{k,n}^{\pm}\}/(2\mathrm{i}d) \\ \mathrm{d}G_k^{\pm}&(x, x', s_k')/\mathrm{d}n_k' \\ &= \pm\sum\nolimits_{n=-\infty}^{\infty}\{(\mathrm{d}x_k'/\mathrm{d}s_k')\,\mathrm{sign}\,(f(x) - f_k(s_k')) \\ &\quad - (\mathrm{d}f_k/\mathrm{d}s_k')(\alpha_{k,n}^{\pm}/\beta_{k,n}^{\pm})\exp[\mathrm{i}Kn(x - x_k'(s_k')] \\ &\quad + \mathrm{i}\beta_{k,n}^{\pm}|y - f_k(s_k')|]\}/(2d) \end{aligned} \tag{2.2}$$

where $\alpha_{k,0}^{\pm} = K_k^{\pm}\sin(\theta)$, θ is the angle of incidence, the wave number $K_k^{\pm} = 2\pi\sqrt{\varepsilon_k^{\pm}}/\lambda_0$, λ_0 is the wavelength in vacuum, $\alpha_{k,n}^{\pm} = nK + \alpha_{k,0}^{\pm}$, $K = 2\pi/d$, d is the period, $\beta_{k,n}^{\pm} = [(K_k^{\pm})^2 - (\alpha_{k,n}^{\pm})^2]^{1/2}$, $\mathrm{Im}(\beta_{k,n}^{\pm}) > 0$; $\mathrm{Im}(\beta_{k,n}^{\pm}) = 0$, $\mathrm{Re}(\beta_{k,n}^{\pm}) > 0$.

The incident field and its normal derivative are given by the expressions:

$$\begin{aligned} \boldsymbol{U}^i &= \exp[\mathrm{i}k^+(\sin(\theta)x - \cos(\theta)y)]\boldsymbol{e}_z \\ \mathrm{d}U^i(s_1')/\mathrm{d}n_1' &= -\mathrm{i}(\beta_{1,0}^{+}\alpha_{1,0}^{+}\,\mathrm{d}f_1(x'(s_1'))/\mathrm{d}s_1') \\ &\quad \exp[-\mathrm{i}\beta_{1,0}^{+}f_1(x'(s_1'))] \end{aligned} \tag{2.3}$$

where $\boldsymbol{e}_z$ is the unit vector along the Z-axis, $f_1(x'(s_{1'}))$ is the function of the first profile; the coordinate $x'(s_1')$ is determined by the curvilinear coordinate s_1' on profile f_1, and the time factor $\exp(-\mathrm{i}\omega t)$ is dropped everywhere.

The amplitudes in the reflected orders can be presented in the following way:

$$\begin{aligned} A_n^{+} = (0.5/d)\int_{S_1}&\{(-\mathrm{i}\beta_{1,n}^{+})(\mathrm{d}U_1(s_1')/\mathrm{d}n_1' \\ &- \mathrm{d}U^i(s_1')/\mathrm{d}n_1') + (\mathrm{d}x'(s_1')/\mathrm{d}s_1' \\ &- (\mathrm{d}f_1(s_1')/\mathrm{d}s_1')(\alpha_{1,n}^{+}/\beta_{1,n}^{+}) \\ &\times(U_1(s_1') - U^i(s_1'))\}\exp[-\mathrm{i}\beta_{1,n}^{+}f_1(s_1') \\ &- \mathrm{i}nKx(s_1')]\,\mathrm{d}s_1'. \end{aligned} \tag{2.4}$$

The efficiencies in the propagating orders are calculated using the expression

$$E_n^{+} = |A_n^{+}|^2\beta_{1,n}^{+}/\beta_{1,0}^{+}. \tag{2.5}$$

The first and the last equations of system (2.1) are single boundary integral equations derived from the expressions for the field in the semi-infinite region 0 and region K, respectively. The two middle equations in system (2.1) are made applicable to all the inner regions by setting appropriately $k = 1, 2, \ldots, K-1$. These integral equations contain boundary integrals coupling the points of observation and integration at neighboring boundaries, as well as the points located at the same boundary. Under certain conditions, Eqs. (2.1) can be replaced by a large system of coupled linear equations containing $2K$ equations and $2K$ unknown electromagnetic field components and their normal derivatives, which can be found, for instance, by blockwise inversion starting with the lowest layer (the corresponding expressions are not presented here because of their being too cumbersome); for more details, see [13]. Eq. (2.1) yields for $K = 2$ an integral equation with one unknown function in the operator form [6].

Joint solution of $2K$ pair equations of system (2.1) is far from being an easy task for modern PCs, even for small values of K and in the resonance region [6,13]. If an X-ray grating consists of many tens of pairs of thin layers, this problem becomes practically intractable for any numerical method [2]. The modified integral method developed by the present author for a bulk grating [10] permits one to cut by an order of magnitude the number of collocation points per boundary, which, considering the cubic dependence of computation time on this parameter, speeds up the calculations about 1000 times. This rate is, however, still not fast enough to allow modeling gratings coated by hundreds of layers, a process requiring staggering amounts of computer time.

The absolute efficiency of an X-ray multilayer grating in the nth order, $E_\mathrm{m}^\mathrm{a}(n)$, was represented [1] by a product of the reflectance of a plane multilayer mirror, $R_\mathrm{m}(\theta')$, by the efficiency of a perfectly reflecting grating $E^\mathrm{p}(n, \theta)$:

$$E_\mathrm{m}^\mathrm{a}(n) = R_\mathrm{m}(\theta')E^\mathrm{p}(n, \theta) \tag{2.6}$$

where $\theta' = \theta$ in a general case, and $\theta' = \theta - \delta$ for a sawtooth-profiled grating with a blaze angle δ (the condition in which the incident ray and the diffraction order n are symmetric with respect to the working groove facet).

In the case of a sawtooth profile, the rigorously calculated efficiency of a perfectly reflecting grating can be replaced by a phenomenological relation based on geometric considerations [1,2]:

$$E^{a}_{m}(n) = R_{m}(\theta-\delta)\min[\cos(\theta-2\delta)/\cos(\theta) \quad \cos(\theta)/\cos(\theta-2\delta)]. \tag{2.7}$$

The numerous rigorous calculations performed by the present author show Eqs. (2.6) and (2.7) to hold with a high accuracy only for low-frequency gratings (300 grooves/mm and 600 grooves/mm) [12].

A fundamental constraint on the application of the above approach for bulk and multilayer X-ray gratings, as well as for gratings with one dielectric coating, is imposed by the oblique angle of incidence, which should not be extremely grazing. For instance, the incidence angle for some bulk gratings should not exceed 40° [1]. The scalar efficiency obtained from Eq. (2.7) was found to differ from that calculated using the rigorous differential method [1] for a multilayer grating working at an incidence angle of 45°. The critical value of the angle depends, however, on the actual grating parameters and the light wavelength and polarization. The incidence angle at which condition (2.7) still holds can in some cases be increased to 70–80° [2]. The limitation on the angle of incidence is connected with the difference in efficiency between the finitely and perfectly conducting bulk gratings operating in the X-ray range under grazing incidence, particularly in the case of the TM polarization. The same applies to multilayer gratings if the radiation penetrates all the way down to the substrate.

Botten [14] proposed a realization of the integral method, which describes light diffraction from a grating with one corrugated surface coated on top and below by several plane transparent layers. Because the fields at the plane layers adjoining the corrugated boundary are related through the Fresnel coefficients, he succeeded in reducing the problem of finding the multilayer grating efficiency to solution of one integral equation at the corrugated surface by modifying Green's functions. The integral method proposed by Botten for the resonance region can be extended to perfectly and finitely conducting reflecting gratings coated by plane layers with complex refractive indices, including those operating in the X-ray range. No such study, however, has thus far been carried out. A comparison of the models underlying determination of the efficiency by Botten and from the product of two reflectances evidences their being similar. The approach of Botten is universal and more precise, compared to a calculation using Eq. (2.6), because it permits one to analyze the efficiency of a grating with a finitely conducting substrate and avoid the limitations associated with large incidence angles.

An approach similar to that proposed by Botten was chosen by the present author for the problem of diffraction from a multilayer X-ray grating, but it was developed along the lines of the first approach, namely, it dealt with the product of the reflectance of a multilayer mirror by the relative efficiency of a finitely conducting grating specified by one (bottom) corrugated boundary:

$$E^{a}_{m}(n) = R_{m}(\theta')E^{a}(n,\theta)/R_{1}(\theta'). \tag{2.8}$$

Our approach is similar to the one based on determination of the field amplitudes found by multiplying the corresponding amplitude scattering matrices. If there is only one corrugated boundary, the calculation simplifies greatly, because the amplitude scattering matrices of a multilayer mirror acquire in this case a trivial form. Realization (2.8) can be employed to advantage in calculation of gratings intended to operate at short wavelengths at different angles of incidence, θ' and θ, on the multilayer mirror and the corrugated boundary, respectively. To adapt the approximate approach to multilayer gratings (2.8), we made use of subprograms developed for bulk grating calculation and for determination of the field amplitudes in reflection from a multilayer mirror [15].

3. Criterion of uncertainty of approximation in calculations of the multilayer X-ray grating efficiency

With the advent of universal numerical methods and the fast progress in computer power and development of various algorithms, the approximate methods (analytical, semi-analytical, and numerical) no longer play a dominant part in theoretical studies. However, approximate approaches can be a help in understanding the physics underlying the complex phenomenon of diffraction and developing a straightforward intuitive approach to its description. This turns out to be particularly important for the X-ray range, where obtaining rigorous solutions to many problems of practical significance still meets with difficulties.

One of the best known among the general approximate methods of solution of diffraction problems in the short-wavelength region is the Born approximation, which provides a fairly high accuracy. The number of the terms to be summed in the Born expansion converging in a small parameter depends on the parameters of the problem and the required accuracy. If the order of the Born approximation (i.e., the number of the terms to be summed up) is large, an exact numerical solution that can be obtained, for instance, by the integral method may turn out preferable. The convergence of a Born series representing the asymptotics of the rigorous solution to an integral equation in the principal diffraction order for the case of one boundary with depth h can be characterized by parameter

$$\xi = (d/\lambda)|\varepsilon^- - \varepsilon^+|(h/\lambda). \tag{3.1}$$

The validity of the Born approximation and estimates of its convergence, similar to Eq. (3.1), as applied to determination of the efficiency of multilayer X-ray gratings with different groove profiles were borne out by rigorous calculations [16]. The condition $\xi < 1$ for the X-ray range is met practically always: $(10^1 \div 10^5)(10^{-1} \div 10^{-6})(10^{-1} \div 10^0)$. The criterion of the accuracy of the results obtained using approximation (2.8) can be gained by substituting the distances S_j between adjacent layers, j and $j+1$, and the angle of incidence θ in Eq. (3.1):

$$\xi_j = (d/\lambda)|\varepsilon_{j+1} - \varepsilon_j|(h/\lambda)(S_j \cos(\theta)/\lambda). \tag{3.2}$$

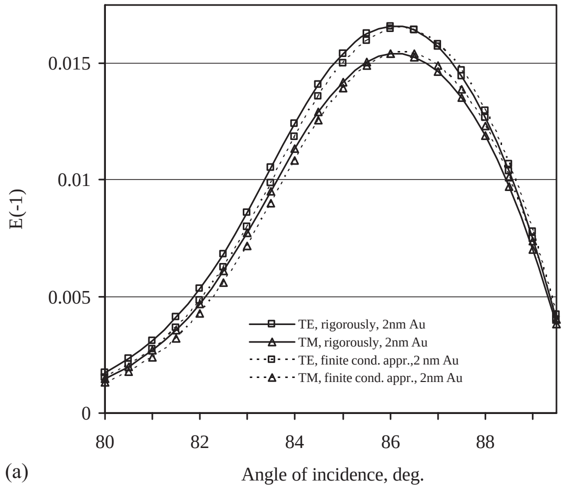
The Bragg condition yields for not too high orders $S_j \cos(\theta)/\lambda < 1$. We choose the condition

$$\xi_j \gtrsim 1 \tag{3.3}$$

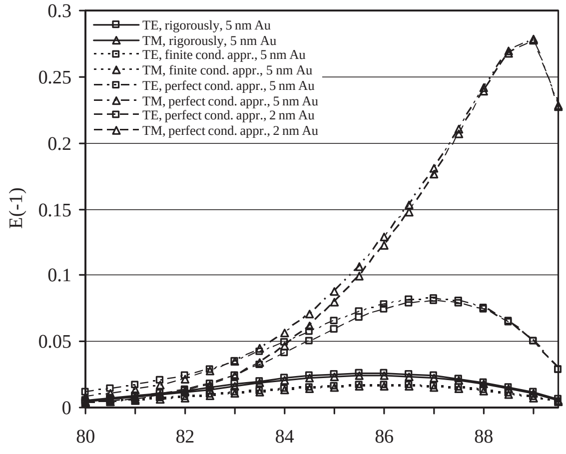
as a criterion of a small uncertainty of results obtained with Eq. (2.8) for grazing-incidence multilayer gratings in the X-ray range.

We can now check the accuracy of approaches (2.6)–(2.8) and the validity of criterion (3.3) by comparing the corresponding figures with the rigorous calculations using Eq. (2.1) of the efficiency of gratings coated by one thin or thick conformal layer and intended for operation in the soft-X-ray range. Consider, as a case in point, a grating with combination of the substrate and layer materials, namely, a silicon sine grating with a groove depth of 11.5 nm, coated by 2 nm of gold, and operating at a wavelength of 5 nm, which corresponds to a maximum efficiency at an angle of incidence of about 86° and a frequency of 3600 groove/mm. In this case, the larger value of parameter ξ_j is 0.09, which fits well to criterion (3.3). The efficiencies obtained for this grating in the—first order by the finite substrate conductivity approximation (2.8) coincide with the rigorously obtained values for both polarizations throughout the angular range covered, up to 89.5° (Fig. 1a). At the edges of the range, the figures coincide to within a few %, and at the maximum near 86°, to not worse than 1%. In contrast to (2.8), approximation (2.6) yields for the TM polarization at incidence angles > 83° a diverging result, which differs from the rigorous figure by tens of times. The efficiencies obtained using approximation (2.6) differ by many times from the rigorous values in both polarizations and throughout the angular range covered (Fig. 1b). The maximum in the efficiency in the—first order calculated for the TE polarization using (2.6) is displaced by approximately 1° relative to its exact position, and its amplitude is approximately five times the rigorously obtained value.

Consider the impact of an increase in the gold layer thickness to 5 nm on the accuracy of efficiency calculation by method (2.8). The convergence parameter (3.2) yields $\xi_j \approx 0.23$, which again satisfies the criterion of obtaining a high-



(a)



(b)

Fig. 1. Efficiency in the—first order of a silicon, sine-profiled, 3600-groove/mm grating with 11.5-nm-deep groove and coated by a 2-nm-thick (a) or 5-nm-thick (a, b) gold layer, calculated vs. angle of incidence for a wavelength of 5 nm.

precision result. The efficiency in the—first order calculated with (2.8) differs for both polarizations by approximately 20% from the rigorous figures, both at the edges and at the maximum (Fig. 1b). The slope of the curves and the position of the efficiency maxima are found by method (2.8) with a much higher accuracy than using (2.6). The results obtained by the perfect substrate conductivity model (2.6) differ by many times from the rigorous figures throughout the angular range under study in both polarizations, to diverge altogether for angles of incidence $>84^\circ$ in the TM polarization. The efficiencies of the Si/Au gratings (Figs. 1a and b) were calculated using 400 collocation points. Correction of the terms in calculation of Green's functions and of their normal derivatives was performed only in the rigorous approach.

As another example, consider the efficiency of a 3600-groove/mm aluminum grating of a 15-nm deep sine profile, which is coated by a 2-nm-thick SiO_2 layer, as a function of the incidence angle at the wavelength of 10 nm. Fig. 2a plots the curves of its efficiency in the—first order, which were calculated by the rigorous (2.1) and the approximate (2.8) approaches for both polarizations in the angular range of 70–89°. The approximate finite-conductivity model offers a good agreement with the rigorous method for both polarizations and throughout the angle range covered, up to 89°. The results obtained for 70° coincide to within four digits after the decimal point, which is comparable to the accuracy of both computations. At the maximum of the efficiency, near 84°, the results obtained with Eq. (2.8) differ from the rigorously obtained figures for both polarizations by not more than 8%. By contrast, the perfect conductivity approximation (2.6) used for the TM polarization and an incidence angle $>80^\circ$ yielded a diverging result, which differed tens of times from the rigorous solution. The efficiencies obtained in this approximation differ from the rigorous figures by a few times for both polarizations, starting from the incidence angle of 70° (Fig. 2b). The maximum in the TE efficiency calculated using approximation (2.6) is shifted to the higher incidence angles by approximately 1.5° with respect to its rigorous position, and its amplitude is three times the exact value. In this particular example, the largest of the two values of parameter ξ_j derived from Eq. (3.2) is about 0.03 near the maximum in efficiency, which fits well to the inaccuracy criterion (3.3).

Let us study the dependence of the accuracy of the results obtained and of estimate (3.3) on the coating thickness. Consider a grating similar to the one just discussed but with a 40 times larger SiO_2 thickness, i.e., 80 nm. The efficiencies of the finitely conducting grating in the—first order calculated

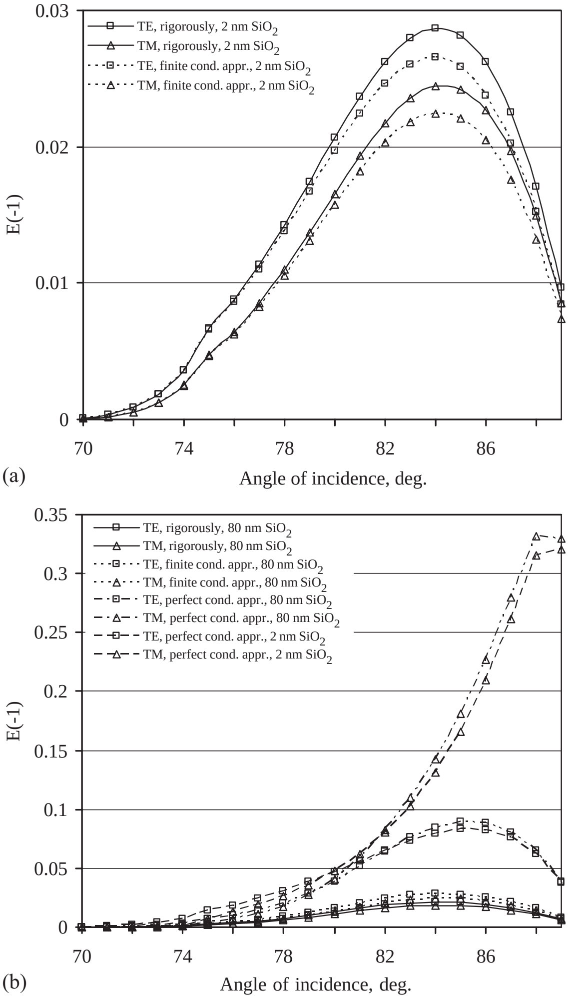


Fig. 2. Efficiency in the—first order of an aluminum, sine-profiled, 3600-groove/mm grating with 15-nm-deep groove and coated by a 2-nm-thick (a) or 80-nm-thick (a, b) glass layer, calculated vs. angle of incidence for a wavelength of 10 nm.

by method (2.8) differ from the rigorous figures by few tens of % at the maximum and at the edges of the wavelength range (Fig. 2b). Despite some quantitative differences, approach (2.8) correctly describes the behavior of the efficiency in both polarizations, including the positions of the maxima and the shape of the curves. The larger of the two values of parameter ξ_j obtained for the angle of incidence of 84° is approximately 1.2, which satisfies the condition of obtaining exact results with (2.8). The efficiency of the Al/SiO_2 gratings (Figs. 2a and b) was calculated using 200 collocation points per one border. The terms in the expansions of Green's functions and of their normal derivatives were corrected only for the results obtained by the rigorous approach.

4. Comparison of the efficiency curves obtained for grazing-incidence multilayer X-ray gratings rigorously, by the approximate approach, and experimentally

A few examples of comparison of theoretical with experimental efficiency curves of typical multilayer X-ray gratings would now be appropriate. The efficiency in the TE polarization of a 1200-groove/mm platinum grating with a 6.195-nm-deep sawtooth profile, coated by 30 pairs of Si/Mo layers 7.32 and 2.3 nm thick, respectively, and operating in the 12.5–14.5-nm range at an angle of incidence of 45° was calculated by the rigorous differential method and in the scalar approximation [1]. The values of the efficiency obtained from the scalar relation (2.7) are inaccurate (Fig. 3), because the angle of incidence is in excess of 40° [1]. Approximation based on (2.8) yields for the

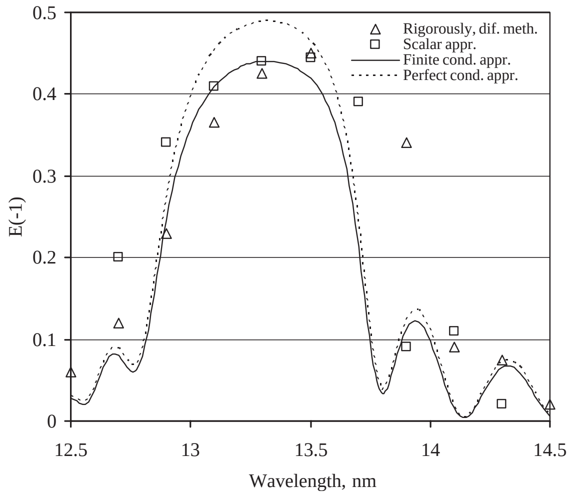


Fig. 3. TE efficiency of a platinum, sawtooth-profiled, 1200-groove/mm grating with 6.2-nm-deep groove and coated by 30 pairs of Mo/Si layers, calculated vs. wavelength for an angle of incidence of 45°.

efficiency in the—first order a value close to the figures obtained by the rigorous differential method. The slight discrepancies in the width of the maximum and the oscillations at the edges of the efficiency curve can be assigned to the lack of precise information on the refractive indices used in the calculation in Ref. [1], because the figures obtained in the calculations from Eq. (2.6) do not coincide at the maximum with the values derived in Ref. [1] using the scalar expression like as (2.7) (Fig. 3). We make use here of the available high-precision values of the refractive indices quoted in [17]. The largest value of parameter ξ_j at $\lambda = 13.5$ nm is about 1.6 for the grating under study, which fits to criterion (3.3). The results obtained using (2.8) are close to those derived rigorously, because the angle of incidence is not grazing. The rigorous differential method [1] imposes a limitation on the grating groove depth, which should not exceed the thickness of the first layer.

Compare now the results obtained by the present author's integral method and the rigorous differential approach, which imposes no constraints on the layer thickness [2]. Consider a gold sawtooth-shaped grating with a period of 360 nm and a blaze angle of 0.5°, which is coated by 30 pairs of Rh/C layers with thicknesses of 1.089 and 2.211 nm, accordingly, and optimized for operation at the wavelength of 1.33 nm [18]. The TE efficiencies calculated from (2.8) coincide with the results obtained by the rigorous differential method to within a few % for most wavelengths (Fig. 4). The calculations made using Eq. (2.6) coincide, on the average, to within 10% with the figures obtained by the differential method, which should be assigned to the small wavelength and the relatively large grazing angle (11.7°).

Fig. 4 plots the efficiencies calculated by methods (2.6) and (2.8) of an X-ray echelle grating with a similar coating and period and operating at 1.33 nm, but with the facet angle of 5° and blazing in the—10th order [18]. The coincidence of these plots with the curve calculated by the differential method is almost as good as in the case of the grating working in the—first order. The agreement obtained with approximation (2.8) is better than that with (2.6), particularly in the left-hand part of

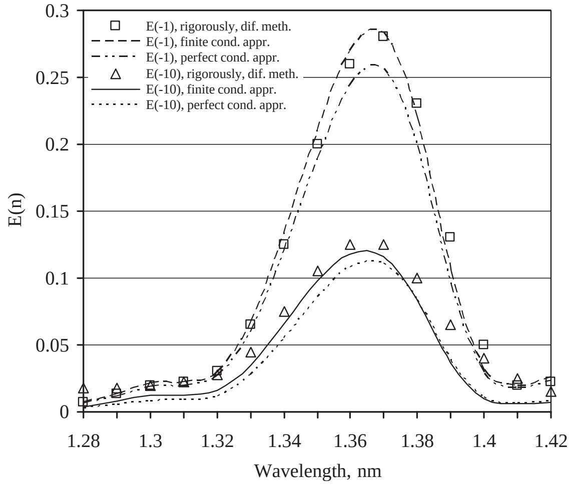


Fig. 4. TE efficiency in different diffraction orders of gold, sawtooth-profiled, 360-nm period gratings with different blaze angles and coated by 30 pairs of Rh/C layers, calculated vs. wavelength.

the curve. Note that the curve in Fig. 4 constructed in the perfect conductivity approximation lies above the finite conductivity curve, while in Fig. 3 the opposite is the case, which implies that method (2.6) is inherently inaccurate. Determination of the echelle grating efficiency is one of the most difficult diffraction problems, which, in addition to the small λ/d ratio and large incidence angles, is characterized by a large grating groove depth. Additional difficulties emerge when studying diffraction on multilayer echelle gratings, particularly in the X-ray range [18]. The high accuracy of the X-ray multilayer echelle efficiency calculations, which was reached with the modified integral method discussed in the paper with modest computational facilities, makes this approach very promising and boosts its potential [18]. The largest values of the ξ_j parameters are 0.76 for a grating with the maximum of efficiency in the—first order and 3.6, in the—10th order. Although the magnitude of ξ_j for an echelle grating exceeds slightly the criterion of obtaining high-precision results, the efficiency in the—10th order is determined with a high accuracy because of the short wavelength. The efficiency calculations for the —first order were performed with 800 collocation points, and those for the—10th order, with 1600 points; besides, in both cases the solution was not refined.

An important check on the grazing-incidence efficiency calculations of multilayer gratings made in approximation (2.8) consists in comparing them with the data derived by the rigorous integral method and in actual measurements. Jark reports on a substantial growth of the efficiency of a grazing-incidence grating in the soft X-ray range reached by applying a multilayer coating [19], but because of there having been no adequate computational program at the time, no comparison with experimental data obtained on a multilayer grating was made. Jark discusses a glass, sawtooth-profiled grating with 1200 groove/mm and a blaze angle of 1.5°, which was coated by an 18-nm-thick gold layer and three pairs of C/Au layers with thicknesses of 11.7 and 6.5 nm, respectively. The grating efficiency in the TE polarization was measured with a reflectometer at fixed radiation lines produced with a Bumble Bee monochromator. The efficiencies in the—first order measured on the multilayer grating in the incidence angle range of 78.5–88° at a wavelength of 5 nm are confronted in Fig. 5a with theoretical data obtained by methods (2.1), (2.6), and (2.8). The data calculated with Eq. (2.8) are seen to coincide practically throughout the incidence angle range covered with the experimental results to within not worse than a few tens of %. The curves calculated by (2.8) and rigorous approaches exhibit a larger difference, particularly in the first maximum region. At the highest grazing angles, the both theoretical curves reveal a tendency to converge. In view of the fact that the calculations were made assuming an ideal groove profile, the difference between the experimental and theoretical values of the multilayer grating efficiency may be considered insignificant. A discrepancy is observed only at non-grazing angles of incidence, where the efficiencies are about 0.001 or less, which is within experimental error, and, hence, can no longer be assumed reliable. The efficiencies calculated with approach (2.6) are larger than those derived from Eq. (2.8) in the beginning and in the middle of the curve by a few tens of %, and at the end of it, by a few hundreds of the same units. Parameter ξ_j reaches its largest value of approximately 1.6 at the

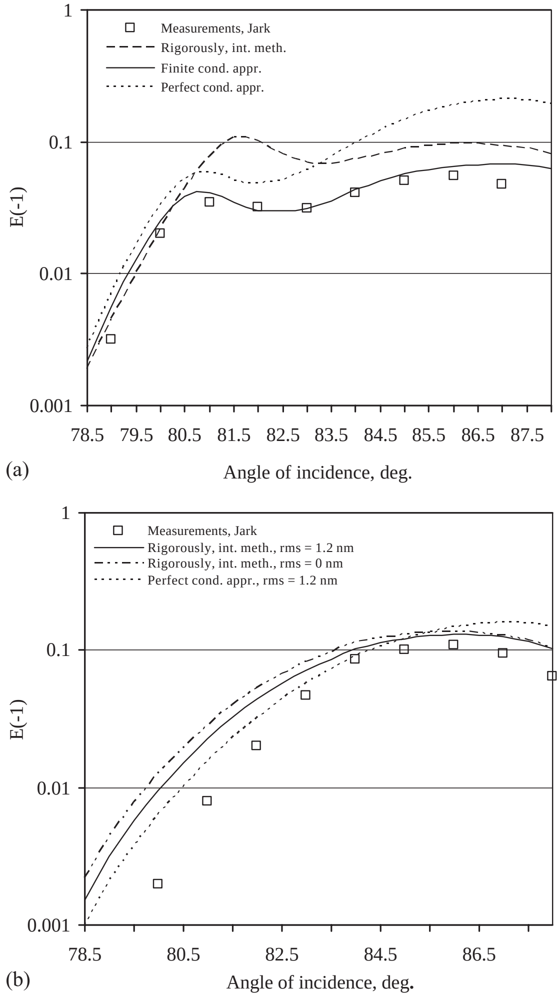
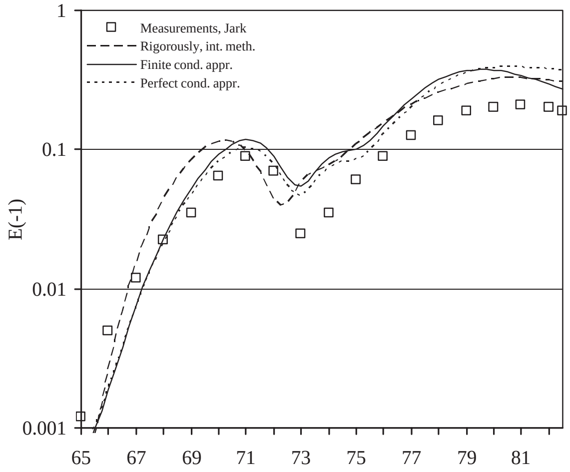


Fig. 5. TE efficiency of a gold, 1200-groove/mm with a blaze angle of 1.5° bulk (b) or coated by three pairs of C/Au layers (a) grating, plotted vs. angle of incidence for a wavelength of 5 nm.

maximum of efficiency near 86°, which fits to criterion (3.3) of obtaining accurate results with Eq. (2.8). The uncertainty of the multilayer Born approximation decrease with decreasing number of layers [16]. Similarly, the smaller inaccuracy of the results obtained by method (2.8) should be assigned to the small number of coating layers. This conclusion is buttressed by the measurements and a rigorous efficiency calculation for a gold grating with the same groove parameters as the multilayer one (Fig. 5b). The difference between the experimental and theoretical values of the efficiency of the gold grating amounts to the same few tens of % in the region of significant values, just as for the multilayer grating. The scatter seen in the bulk grating efficiencies should be attributed to the only cause, namely, to using the ideal groove profile shape in the calculations. The results obtained by the rigorous differential method for the gold grating and rms roughness $\sigma = 0$ [20] coincide in Fig. 5b, within the plotting accuracy, with the theoretical figures derived by the rigorous integral method.

The efficiencies in the—first order measured on the multilayer and the bulk gold grating in the incidence angle range of 65–82.5° at a wavelength of 10 nm are confronted with theoretical data (Figs. 6a and b). The efficiencies calculated from Eq. (2.8) are applicable not only qualitatively but quantitatively for this case as well. The values obtained by approach (2.8) and by the rigorous approach coincide to within not worse than a few tens of % throughout the incidence angle range covered despite of some shift in the maximums positions. The calculated and measured results exhibit a larger difference. Just as for the wavelength of 5 nm, the major reason for the discrepancy between the experimental and theoretical data on the efficiency for the wavelength of 10 nm is not the large value of the parameter $\xi_j = 1.8$ but rather the use of the ideal grove profile in the calculations. This conclusion is supported by an analysis of the discrepancies between the measured and calculated efficiencies of the gold grating (Fig. 6b). The experimental and theoretical efficiencies of the bulk and multilayer gratings disagree noticeably in the central part of the curves while converging at larger incidence angles (Figs. 6a and b). The gold grating efficiencies obtained by the rigorous integral method agree, within the plotting accuracy, with the data yielded by the rigorous differential method [20] for an rms roughness $\sigma = 0$ nm (Fig. 6b). The—first order efficiencies of a multilayer grating calculated for the wavelength of 10 nm by method (2.6) exhibit a larger disagreement with the measurements compared with the modeling by (2.8), particularly for large angles of incidence (Fig. 6a), just as in the case of the 5 nm wavelength. The efficiencies of the Au and Au/C gratings for the both wavelengths



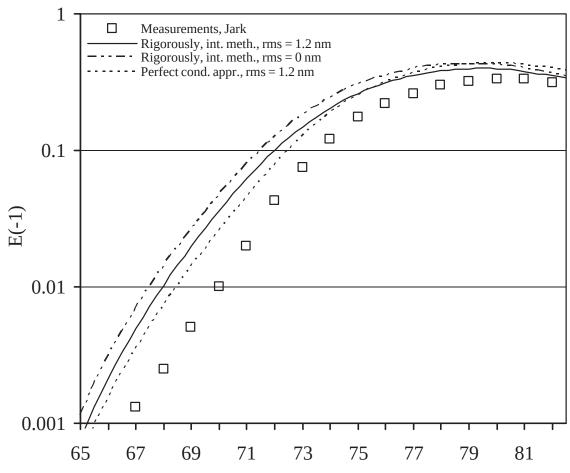


Fig. 6. TE efficiency of a gold, 1200-groove/mm with a blaze angle of 1.5° bulk (b) or coated by three pairs of C/Au layers (a) grating, plotted vs. angle of incidence for a wavelength of 10 nm.

were calculated using 400 collocation points. Correction of the terms in calculation of Green's functions and of their normal derivatives was performed only in the rigorous approach.

5. Conclusion

Rigorous approaches to modeling multilayer-coated X-ray gratings meet with considerable numerical difficulties, while invoking the scalar theory of diffraction or application of the perfect conductivity approximation fails to yield exact results, particularly for grazing incidence angles, in the TM polarization, and in high orders. The proposed approximation to the rigorous integral method permits one to obtain with a high precision the values of efficiency over a broad range of parameters of X-ray gratings, including those with a real (AFM-measured) groove profile shape. It is independent of the number of layers and can be used on a standard PC. The approximate approach is capable also of taking readily into account layers with roughnesses of various kinds and their mutual diffusion. A criterion of the accuracy provided by the approximation to the integral method for multilayer X-ray grating efficiency calculations was proposed, and the conditions of its application were analyzed. A good agreement was obtained in all multilayer grating cases with an accuracy not worse than that reached for equivalent bulk gratings. The efficiencies of multilayer gratings measured at grazing angles with synchrotron soft X-ray radiation are in good agreement with the values calculated using the integral method for ideal groove profiles. The rigorous and the approximate approaches have been integrated into the PCGrate®-SX program used to obtain the results presented in this paper.

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