Rigorous efficiency calculations for blazed gratings working in in- and off-plane mountings in the 5–50-Å wavelengths range

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ABSTRACT

Both classical (in-plane) and conical (off-plane) grating configurations can be used in the spectrometer being developed for the Spectroscopy X-ray Telescope (SXT), which is assigned for the Constellation-X mission. Rigorous absolute efficiency calculations of gold-coated diffraction gratings with ideal triangular, trapezoidal, and polygonal profiles have been carried out for both possible spectrometer mountings by the PCGrate®-SX program based on a modified integral method, with due account of random roughness. Optimum grating parameters and spectrometer configuration providing maximum theoretical efficiency were determined. Rigorous calculations performed with optimization showed that blazed grating absolute efficiency for the in-plane configuration similar to that employed in the XMM-Newton X-ray telescope cannot exceed 0.2–0.3 at the maxima in the minus first diffraction order within the relevant range of grazing angles, frequencies, and blaze angles. By contrast, using a grazing off-plane mounting permits one to compute gratings with a few times higher theoretical absolute efficiency in first diffraction orders, both at the maxima and on the average, for much higher grating frequencies and blazing angles. Unlike the classical mount, conical diffraction gives rise to noticeable polarization effects and Rayleigh anomalies in TM polarization. In view of the possibility of fabricating almost ideal triangular grooves by anisotropic etching of smooth graze-cut (111) silicon wafers by interference lithography and of compensating aberrations by properly modifying the frequency and/or grating groove curvature, the off-plane grating configuration may turn out preferable, particularly if a high spectral resolving power can be reached. A comparison with efficiency calculations and measurements is presented.

Keywords: diffraction grating, x-ray spectroscopy, conical mounting, integral method, rigorous efficiency calculations

1. INTRODUCTION

Being a part of the Spectroscopy X-ray Telescope (SXT) on the Constellation-X mission, the reflection grating spectrometer (RGS) is intended for operation in the softest x-ray region of 0.25–2 keV with a high spectral resolving power and efficiency[1]. For instance, measurement of *K*-shell x-ray lines requires a resolving power of a few thousands, and to reach the goal of the telescope effective area[2], the gratings have to have an efficiency of about 0.5.

The baseline reflection grating spectrometer design involves an array of thin reflection gratings mounted at grazing incidence to the beam immediately behind the Spectroscopy X-ray Telescope optics. Thin grating plates measuring 100 × 200 mm are combined in blocks of 10 each, which are integrated in several tens of RGS flight modules. The thin grating films are bonded to stiff carrier frames under tension and positioned within an assembly structure using precision four-point mounts within the assembly structure. The integrating structure supporting the grating array is integrally coupled to a deep, stiff telescope structure, that also supports the mirror shells. The light picked off by the gratings is dispersed to a strip of CCD detectors offset in the dispersion direction. The gratings are all mounted at the same incident graze angle with respect to the ray passing through grating center, and they are positioned on a Rowland torus, which also bears the telescope focus and the CCD detectors. This configuration eliminates the comatic aberrations due to the convergence of the beam intercepted by each individual grating, through slight variation of the groove spacing or curvature over the length of the grating.

The grating spectrometer for the Constellation-X mission can be designed by either of the two geometries, more specifically, the in-plane and off-plane ones. The in-plane mounting is similar in design to that used in the XMM-Newton X-ray telescope[3]. To improve the XMM heritage, the reflection gratings were fabricated by interference lithography on graze-cut (111) silicon wafers. This concept exploits the highly anisotropic etching property of special silicon etches, which stop at the (111) lattice planes and, thus, effectively produce grating grooves with atomic

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smoothness and a high degree of geometry control[4]. While any other appropriate technology can be employed in grating fabrication, holographic technique demonstrates obvious advantages. Irrespective of the technology used to fabricate a master or a replica grating, they should be coated by a layer of gold or another noble metal to enhance reflection, the goal being to reduce roughness down to rms <5 Å. In-plane gratings designed for operation in the soft x-ray range have typically a low groove frequency and an extremely small blaze angle[5]. Off-plane gratings should have high frequencies (5000 gr/mm and more) and relatively large blaze angles (~10°)[5]. The off-plane arrangement provides, as a rule, a resolving power comparable to that reached in the in-plane mounting[5]. However, if the telescope spatial resolution and high orders are duly taken into account[2,6], the resolving power of the off-plane mounting under study here can even be higher.

Such severe, previously unattainable requirements on the grating unit of the spectrometer for the Constellation-X mission set special requirements on the design of the gratings and the technology of their fabrication and testing. To reach the maximum possible spectrometer throughput, the parameters of the grating have to be optimized with due account of the technology of its fabrication and the operational scenario. Recall that the absolute efficiency predicted by scalar methods may differ by a few times and even tens of times from the figures obtained by rigorous numerical techniques or measurements[7,8]. This communication reports on a rigorous method of analysis (more specifically, a modified integral method[9]) by the PCGrate®-SX computer program of the theoretical efficiency of gratings designed for operation in both the in- and off-plane RGS mountings.

2. VALIDATION OF THE METHOD AND RELEVANT SOFTWARE

Modeling of diffraction grating efficiencies in the short wavelength range by rigorous vector theories has until recently been a cumbersome task even with the presently available large memory and high speed of modern computers. In the soft x-ray–EUV range, correct account of shading, absorption, polarization effects, roughness, and other electromagnetic properties of the grating is required, along with that of the extremely small values of the wavelength-to-period ratio. Reliable absolute efficiency predictions for relief gratings working in these spectral regions have become possible only after the development of such efficient numerical methods as the differential[10,11], modal[12-14], and integral[8,15]. Rigorous calculations based on the first two approaches deal with ideal groove geometry profiles. Of most interest for this wavelength region is, however, to model gratings with a real groove structure, which can be done by the method of integral equations. For instance, the IESMP[16] and modified integral[17] methods are capable of handling gratings with real groove profiles measured by AFM or any other modern tool[18,19]. In contrast to the IESMP, the modified integral method uses in soft x-ray computations an order-of-magnitude smaller number of discretization points for approximately the same output accuracy[16,17]. This is a substantial advantage in view of the computation time and the required operating memory depending in the IESMP[16] quadratically on this parameter. In addition, the present-day realization of the modified integral method provides a possibility of taking into account random interface roughness, calculating various off-plane diffraction designs, and modeling concave gratings[20].

We are going to illustrate the potential of the modified integral method and the accuracy provided by the corresponding program with two examples to compare the relevant data with the figures obtained for the grating efficiency in soft x-rays and XUV by other rigorous methods and computer codes. As the first example, we take the calculated and measured efficiencies of the plane gold-coated diffraction grating in the BESSY II monochromators, which operates in a grazing-incidence in-plane mounting in the fixfocus (fixed ratio of the cosine of the incidence angle to that of the minus first order diffraction angle) condition over an energy range extending from 50 to 1100 eV[8]. The 1200-gr/mm grating works at a constant fixfocus of 2.25 and has a sawtooth groove profile (90° apex angle) with a blaze angle of 1.3°. The gold refractive indices were taken from Ref. 21.

Figure 1 displays plots of the absolute efficiency in unpolarized light obtained for this grating in the 0 and –1 orders by direct measurements and computations making use of three rigorous codes, namely, IESMP, LUMNAB[8], and PCGrate®-SX[20]. As seen from Fig. 1, the results obtained by all the three computer methods differ from one another at the corresponding points by about a few relative percents, with the exception of the last point at 1100 eV. The difference of the PCGrate®-SX from LUMNAB results for this point is as high as about 8 relative percents, which may be assigned to the insufficiently accurate representation of the groove profile made in the differential method[8]. The overall good agreement of all results obtained by three different approaches in this fairly difficult case for computations provides reasonable grounds for confidence in the corresponding programs. Note that all computations performed with the PCGrate®-SX used 400 discretization points, and a Dual Intel® Pentium III®, 1 GHz, 256 KB Cache Workstation computer with a 1024 MB RAM and 133 MHz Bus Clock working under MS® Windows 2000 Pro® takes one min per point on the plot, with due account of the paralleling and caching. As for a certain difference between the calculated and measured data on the efficiency, they should be assigned primarily to the theoretical model constructed for the groove profile. It is known[16,18,20] that idealization of the groove profile may entail errors on the order of a few tens and more of relative percents in the minus first order. Still larger deviations are observed to occur in higher orders[8].

As another example of comparison, consider the calculated efficiency of a gold sawtooth-shaped grating with 3600 gr/mm and a blazing angle of 5°, which operates in unpolarized light under grazing incidence and off-plane diffraction in the direction of the rulings at a wavelength 13.34 Å[22]. The PCGrate®-SX program was employed to calculate the efficiency in the 0, –1, and –2 orders under a polar (the dispersion plane) angle of incidence of 5° as a function of the azimuth (off-plane) incidence angle. The gold refractive index used in the calculation was taken from Ref. 23.

Figure 2 plots the absolute efficiency of this grating calculated in three diffraction orders together with the total reflected energy curve. We readily see that the results obtained[22] by the differential method practically coincide with those made by the present author. All the computations performed with the PCGrate®-SX program made use of 400 discretization points, and obtaining one point in the plot, including the use of the invariance theorem[24], paralleling, and caching, takes up less than 13 s of time on the above-mentioned computer. Figure 2 does not display the data of the corresponding efficiency measurements reported in the pioneering work[25]. These experimental data turned out to be several times smaller than the theoretical figures because of the poor quality of the grating tested[25]. As follows from the typical curves presented in Fig. 2, with a fixed azimuth angle of incidence the relative efficiency at the maxima in the first two off-plane diffraction orders is in excess of 0.9. The absolute theoretical efficiency in a given order is determined for a given material by the wavelength and groove profile shape[26]. This dependence is dealt with in Sec. 4 of the present study.

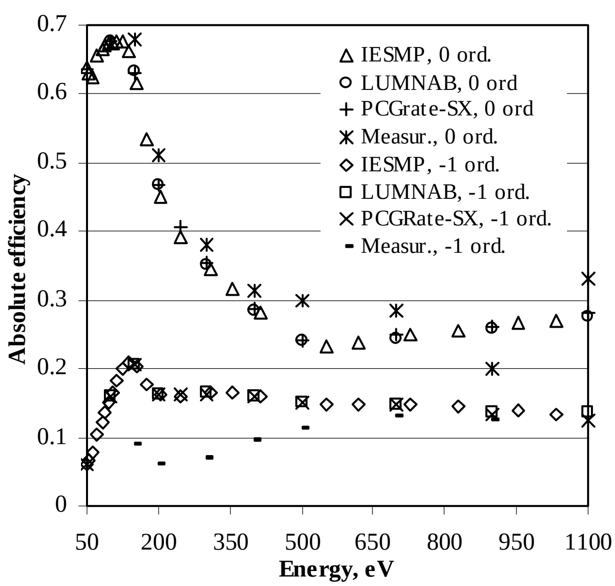

Fig. 1. Absolute efficiency in the 0 and –1 orders of a 1200-gr/mm sawtooth grating with 1.3° blaze angle and 2.25 fixfocus plotted as a function of energy for the in-plane mounting.

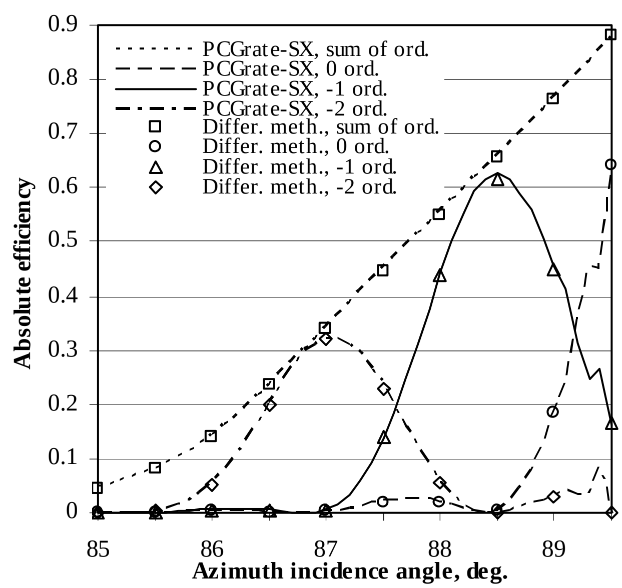

Fig. 2. Absolute efficiency in the 0, –1, and –2 orders of a 3600-gr/mm sawtooth grating with 5° blaze angle calculated for a 13.34-Å wavelength incident at 5° polar angle as a function of azimuth incidence angle for the off-plane mounting.

3. IN-PLANE MOUNTING

To illustrate the in-plane mounting, we shall determine now the optimum parameters and calculate the highest attainable absolute diffraction efficiency of a gold-coated sawtooth grating with 1000 gr/mm using our PCGrate®-SX computer program. As follows from the blaze condition for this grating and the value of the critical angle for gold obtained with the relevant refractive indices[27], this groove frequency is actually the limiting value still providing noticeable light diffraction in the –1 order near 5 Å. Consider the dependence of the absolute efficiency of a diffraction grating on light incidence angle and its blaze angle assuming the groove to have an ideal profile and a gold surface roughness rms = 10

Å. The accuracy parameter for all calculation was 400 discretization points, and in these conditions the total error derived from the energy balance does not exceed for almost all points 0.001.

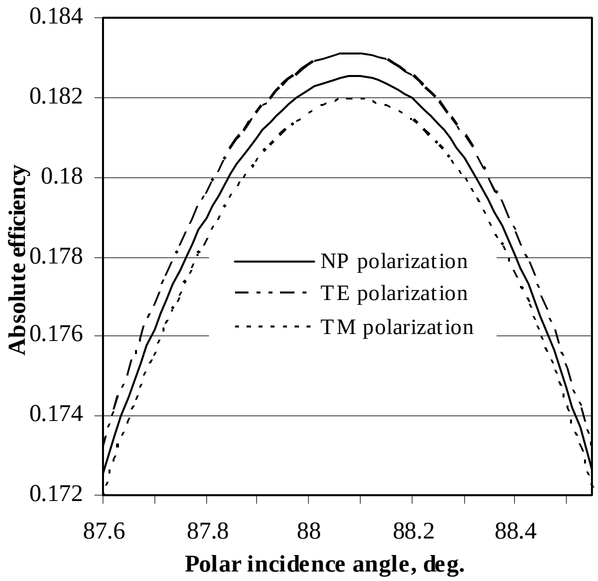

Fig. 3. Absolute –1 order efficiency of a 1000-gr/mm sawtooth grating with 0.9° blaze angle and 10-Å rms roughness calculated for a 15-Å wavelength as a function of polar incidence angle for the in-plane mounting.

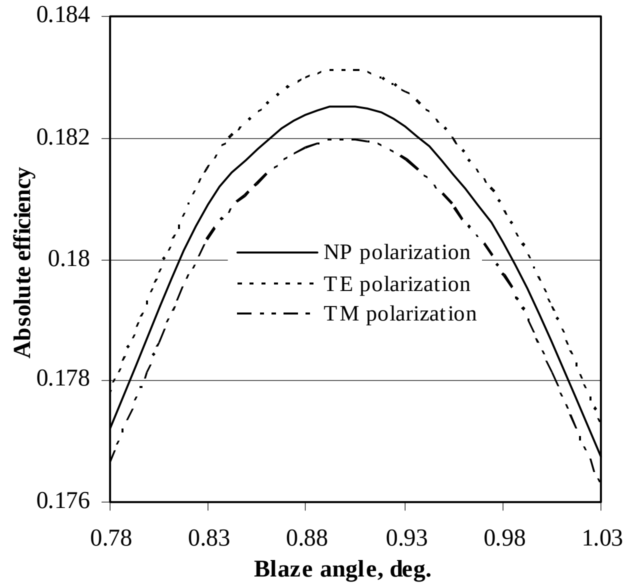

Fig. 4. Absolute –1 order efficiency of a 1000-gr/mm sawtooth grating with a 10-Å rms roughness calculated for a 15-Å wavelength incident at a 88.1° polar angle as a function of blaze angle for the in-plane mounting.

Figure 3 presents the absolute efficiency of the grating under study in the –1 order plotted against polar incidence angle in the interval 87.6–88.55° for an optimal blaze angle of 0.9° and a wavelength 15 Å, and for the TE, TM, and NP (non-polarized light) polarizations. As evident from Fig. 3, all the three curves pass through a smoothly sloping off maximum near 88.1°, with only a weak effect of polarization being manifest. Figure 4 displays similar curves illustrating the dependence on the blaze angle in the interval 0.78–1.03° obtained under an optimum incidence angle 88.1° and a wavelength of 15 Å. The blaze angle dependence exhibits the same smoothly decaying character, with the maxima in the same positions and only a small difference in efficiency for different polarizations seen. The maximum in diffraction efficiency about 0.182 observed in both these figures is the maximum predicted by theory for this grating, whish is optimized for the 15-Å wavelength. These curves are actually nothing else but perpendicular sections of the three-dimensional –1 order efficiency surface constructed by rigorous calculations. Note also that even a significant deviation of the apex angle from 90° does not practically affect the efficiency in the –1 order.

Figure 5 plots the dependence of efficiency on wavelength calculated for the three first diffraction orders in the 5–50-Å region for a grating with a blaze angle 0.9°, which operates at an incidence angle of 88.1°, i.e., under the conditions optimal for the wavelength of 15 Å. As seen from Fig. 5, the difference in the –1 order efficiency between two perpendicular polarizations planes varies from a few tenths of a relative percent to a few relative percents, a value of no practical significance at all. The efficiency difference obtained for different polarizations in higher orders is too small to be discerned in the plots, and is not shown in the Fig. 5. By contrast, as evident from the –1 order efficiency curve presented for comparison in the same figure for a grating with zero roughness, roughness with rms = 10 Å affects strongly the efficiency in the principal (and other) order(s) by reducing it by a few tens of relative percents at the short-wavelength edge. Note also the very low efficiencies in higher orders even at the shortest wavelengths considered. Obviously enough, to improve the efficiency in the –2 or –3 orders, one will have to optimize the incidence and blaze angles for the corresponding order, with due account of the wavelength.

Figure 6 plots the efficiency vs. wavelength in the 5–50-Å range for three first diffraction orders of a gold sawtooth 641-gr/mm grating with a blaze angle of 0.75°, which operates at an incidence angle 88.43° in the RGS on the XMM-Newton X-ray telescope[3]. As with the 1000-gr/mm grating, the calculations were performed for the refractive indices taken from Ref. 27 and roughness rms = 10 Å. The RGS grating on the XMM telescope has a maximum of the –1 order also near 15 Å, and it exhibits a still smaller difference in efficiency for different polarizations. A rigorous efficiency calculation of the XMM telescope RGS gratings with other parameters was obtained by the differential method[7] neglecting random roughness. As follows from a comparison of Figs. 5 and 6, the absolute grating efficiency in the –1 order, and, particularly, in higher orders, increases with grating period. For instance, the efficiency of the XMM grating at the maximum in –1 order exceeds that of the 1000-gr/mm grating by 36 relative percents, which is proportional to the difference in the periods. The efficiency in the –2 order of the XMM grating is more than twice that in the corresponding order of the 1000-gr/mm grating, and the efficiency in the –3 order exceeds that more than tenfold. Such large differences suggest a need of optimizing the groove profile parameters and incidence angle based not on the optimal parameters for the –1 order only.

In conclusion to this Section, compare the main results obtained here by rigorous calculations for a classical mounting with the predictions of scalar theory of diffraction. It can be readily verified that the optimal parameters of low-frequency gratings which are applicable to this range with a high accuracy can be derived, as the absolute efficiency at the maximum itself, from straightforward geometrical considerations[7,10,28,29]. For instance, the value of the maximum theoretical efficiency for the 1000-gr/mm grating obtained on scalar grounds differs by 7 relative percents only from the result of rigorous calculations. The points on the efficiency curve far from its maximum in the –1 order cannot, however, already be predicted on the grounds of scalar theory. As for the higher orders, the efficiencies derived from simple geometric expressions can differ by a few and even tens of times from the precise calculated figures[7,8]. The increase of diffraction order acts in the same way on efficiency calculations as that of the grating period[10,28,29], indeed, the larger are these two parameters, the less scalar is the efficiency behavior. If, however, calculations have to take into account the real groove profile, the efficiency of even low-frequency gratings cannot be determined in any diffraction order without invoking rigorous methods[8,16–18,20].

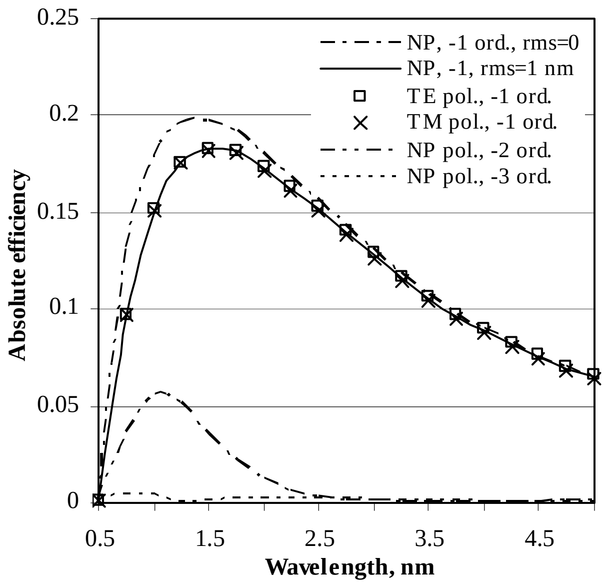

Fig. 5. Absolute efficiency in the –1, –2, and –3 orders of a 1000-gr/mm sawtooth grating with 0.9° blaze angle calculated as a function of wavelength for the 88.1° polar incidence angle and the in-plane mounting.

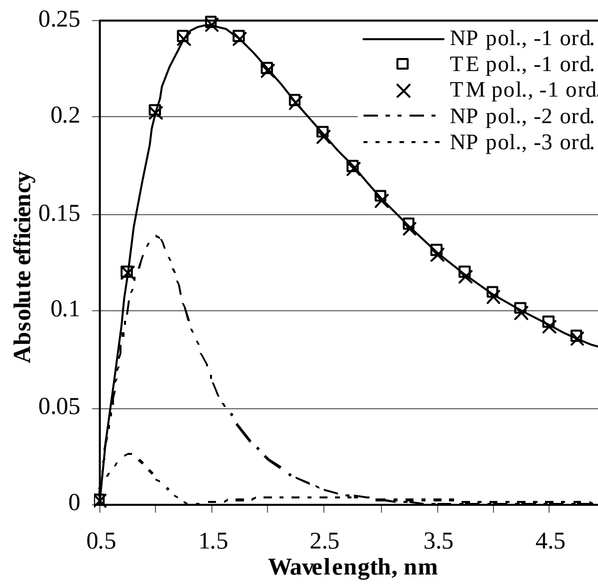

Fig. 6. Absolute efficiency in the –1, –2, and –3 orders of a 641-gr/mm sawtooth grating with 0.75° blaze angle and 10-Å rms roughness calculated as a function of wavelength at the 88.43° polar incidence angle and the in-plane mounting.

4. OFF-PLANE MOUNTING

We selected for illustration of absolute efficiency calculations for the case of grazing-incidence, off-plane mounting operation gratings with 5000 and 6000 gr/mm and profiles of three types, namely, triangular, trapezoidal, and polygonal. As follows from the blaze condition for a grating working in off-plane mounting[26] and the values of the critical angle for gold with refractive indices taken from Ref. 27, the high groove frequency should be complemented by a large enough blaze angle to obtain maximum efficiency at the short-wavelength end of the operating range. The theory of conical diffraction is treated in considerable detail, e.g., in Ref. 24. The large depth of the gratings combined with the small number of propagating orders under grazing off-plane diffraction gives rise to appearance of strong polarization effects and anomalies in the spectral response of TM efficiencies in the various orders. Note that linearly polarized light incident under off-plane diffraction conditions on a finitely conducting grating becomes elliptically polarized. In addition, the groove profile (depth) and grazing incidence angle exert strong influence in this operating mode on the shape and magnitude of the efficiency curves. All these features in the behavior of efficiency cannot be established, even approximately, without invoking rigorous numerical methods[26]. In this Section, the author is going to study the behavior of the efficiency of off-plane diffraction gratings with an ideal and a close-to-realistic groove profile for a range of close-to-grazing azimuth incidence angles and random roughnesses. All calculations were performed using the same PCGrate®-SX program, and the accuracy parameter was 200 discretization points. The total error for all points derived from the energy balance[17] does not exceed 0.0001, and the time taken up to calculate one point with the specified computer is about 2 s.

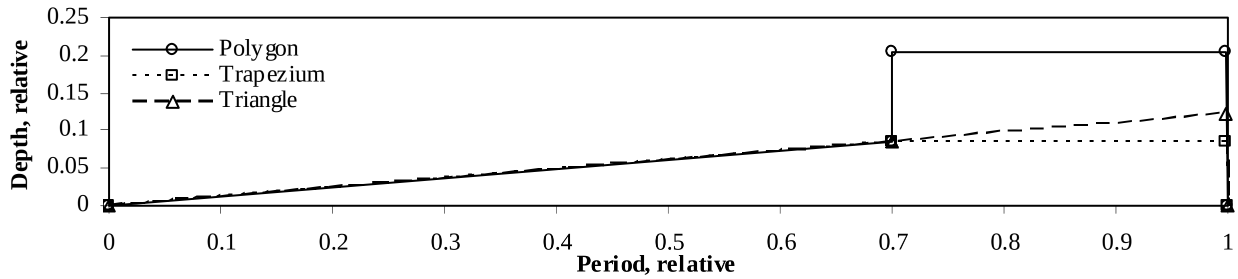

Fig. 7. Groove profile function of the polygon, trapezium, and triangle plotted in units of the period.

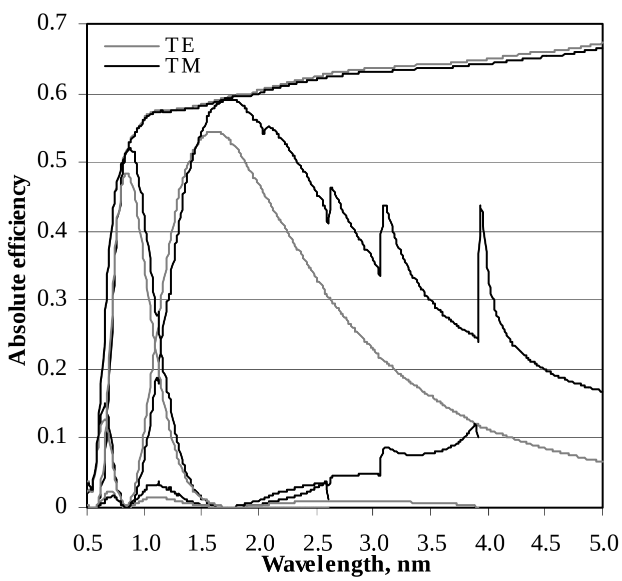

Fig. 8. Absolute efficiency in the –1, –2, and –3 orders of a 5000-gr/mm triangular grating with 7° working facet angle and 5-Å rms roughness calculated as a function of wavelength for the 7° polar and 88° azimuth incidence angles and the off-plane mounting.

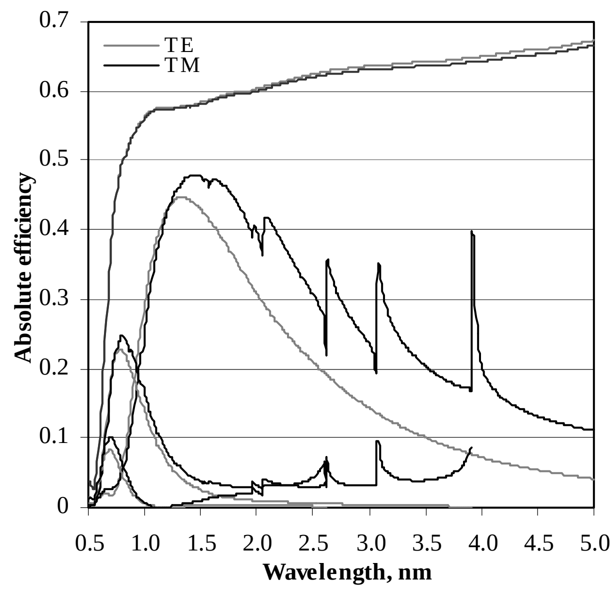

Fig. 9. Same as in Fig. 8 but for a trapezoidal grating.

Figures 8–13 present plots of the absolute efficiency vs. wavelength of 5–50-Å incident radiation polarized in two perpendicular planes (TE and TM), which were calculated for the three first negative diffraction orders, and of the total energy reflected from gold-coated 5000-gr/mm gratings with grooves of three types depicted in Fig. 7. The working facet angle is 7°, and the width of the flat top of the trapezoid or nub of the polygonal profile constitutes 0.3 period. The depth of the polygonal profile, as determined by least-squares fitting the calculated efficiency in the principal order to the respective measured efficiencies (see table), is 0.205 period. The polar incidence angle (in the dispersion plane) is 7° for all gratings, i.e., the projection of the wave vector on this plane is perpendicular to the working facet[24,26]. The azimuth angle of incidence is 88 or 88.5°. The groove parameters chosen for the modeling are close to the real figures for the gratings fabricated by the presently most advanced technology of selective etching of single-crystal silicon plates and the techniques accepted for the measurement of their efficiency[30, 31].

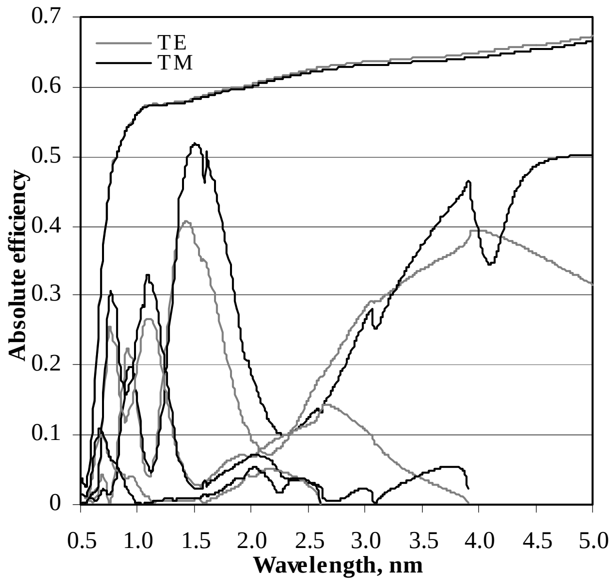

Fig. 10. Same as in Fig. 8, but for a polygonal grating.

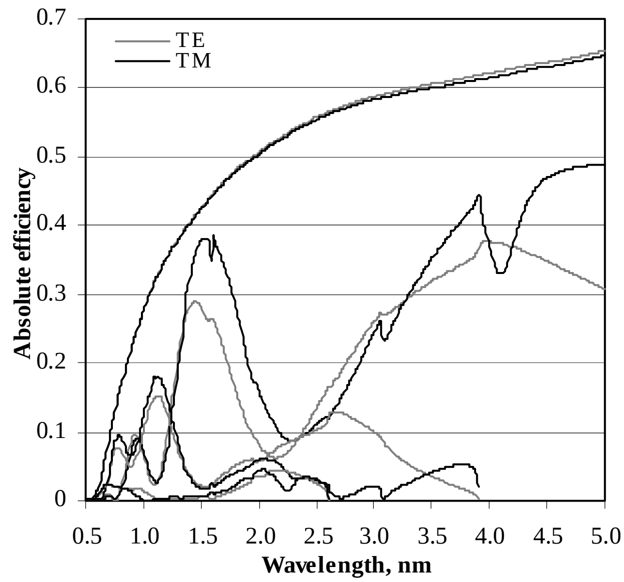

Fig. 11. Same as in Fig. 8, but for a polygonal grating with rms roughness of 20 Å.

Although the apex angle of the triangle etched by this technology is 70.53°, the real profile differs from the ideal one, a conclusion supported by its SEM image.[30] Therefore our calculations made use of profiles with a vertical non-working facet. Note that varying the apex angle within a certain range does not practically affect the efficiencies in the first diffraction orders.

As evident from Figs. 8–15, gratings operating under the conditions of grazing off-plane diffraction exhibit strong polarization properties, particularly for the triangular groove geometry. The difference between the TE and TM component efficiencies is particularly large in the vicinity of the Rayleigh wavelengths, where the behavior of TM efficiencies in various orders show strong anomalies when one of them disappears. As seen from Fig. 8, the efficiency in the –1 order (the one with the highest maximum) calculated for the TE and TM components near 39 Å differs by nearly a factor four for the grating with triangular grooves and an azimuth incidence angle of 88°. In higher orders, this difference may be as high as tens and even hundreds of times, with the efficiency in one of the components (TE) being extremely low. Besides, the TM efficiency maximum in the –1 order is shifted noticeably in position to longer wavelengths compared to the TE efficiency peak. Another feature seen from Fig. 8 is that the chosen profile and incidence angle parameters are close to optimal (compare with Fig. 2) for the –1 order and a wavelength near 16.6 Å. Figures 9 and 10 display efficiency curves with the same parameters as in Fig. 8 but calculated for the trapezoidal and polygonal gratings, accordingly. As seen from a comparison of Figs. 8 and 9, the truncation of the triangular profile observed to occur as one goes over to the trapezoidal shape affects negatively the efficiency, both at the maximum and spectrally averaged, particularly for high orders. Indeed, the efficiency in the –2 diffraction order (the one with the second smallest amplitude in the graphs) of the trapezoidal grating is lower than one half that for the triangular grating in both polarizations. Besides, the width and magnitude of the Rayleigh resonances of the TM component change, while the efficiency curves preserve their general pattern. The shape of the efficiency curves changes dramatically for all orders as one goes over to the grating with the polygonal profile (Fig. 10). The nub in the profile gives rise to several oscillations and a strong energy redistribution between the –1 and –2 orders in the short-wavelength part of the curve. In the long-wavelength domain, one observes an anomalous growth in efficiency compared to the triangular and trapezoidal gratings, including the TE component, which stops only near 45 Å. Note that while the TM efficiency likewise exhibits resonances, they become substantially broader and smaller in amplitude. It should be pointed out that the average efficiency in the –1 order and the average sum of efficiencies in the first three orders calculated for a grating with polygonal profile in the short-wavelength and medium parts of the operating range are noticeably lower than those for the gratings of the other two profiles.

The curves in Figs. 8–10 were calculated under the assumption of the presence of random roughness with rms = 5 Å, which is the goal for the RGS of the Constellation-X mission and does not bring about a noticeable decrease in reflection in the short-wavelength part of the operating range. An analysis of the experimental values of total energy reflected in all orders[31], as well as an extensive modeling of the effect the parameters of the various profile shape exert on the efficiencies in the main orders, which was performed by the present author, suggest that the real rms roughness may be as high as a few times the measured value[30], or that the measurements of reflected energy are not accurate enough. Figure 11 presents calculated efficiency in the main orders of a polygonal-groove grating with an rms roughness of 20 Å. This plot differs from the one in Fig. 10 only in lower reflection figures at the short-wavelength edge. This proportional decrease in the efficiency in all orders is about seven times for 6 Å, two times for 10 Å, and 27% for 15 Å.

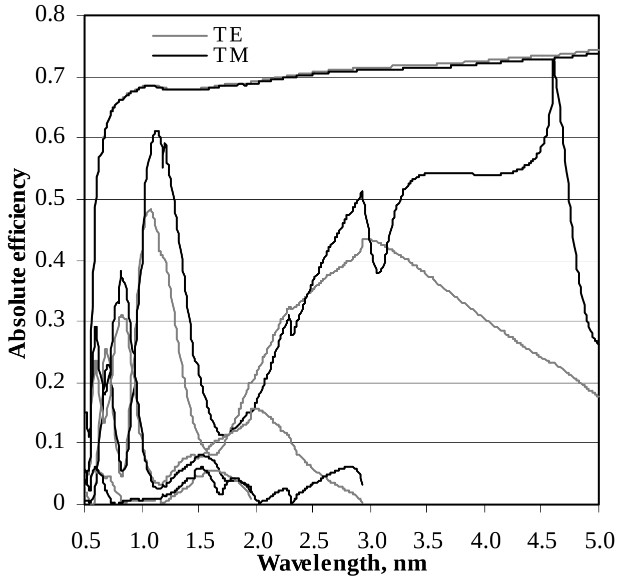

Fig. 12. Same as in Fig. 8, but for a polygonal grating and an azimuth incidence angle of 88.5°.

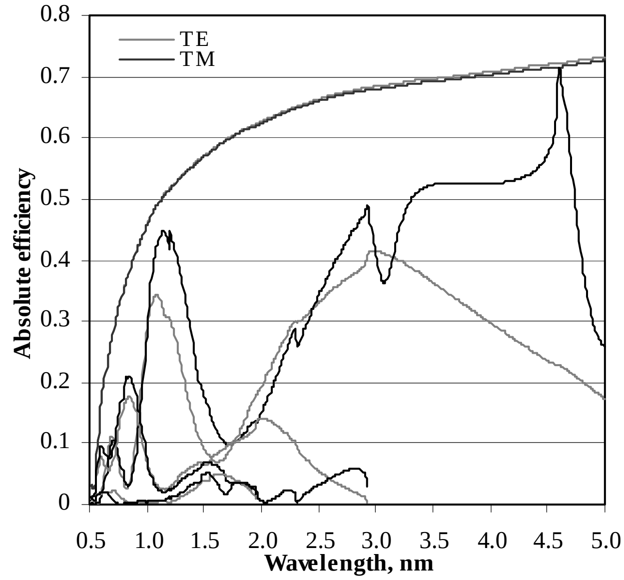

Fig. 13. Same as in Fig. 8, but for a polygonal grating with rms roughness of 20 Å and an azimuth incidence angle of 88.5°.

Figures 12 and 13 present efficiency curves calculated for a polygonal grating operating under an azimuth incidence angle of 88.5° and having an rms roughness of 5 and 20 Å, respectively. Compared with the similar curve in Fig. 10 calculated for an azimuth angle of incidence of 88°, the efficiencies in the –2 order depicted in Fig. 12 are tens of times higher than the values in Fig. 10 at the very edge of the short-wavelength range. Both the maximum and the average efficiencies in the principal order obtained for the azimuth incidence angle of 88.5° exceed those calculated for the angle 88° throughout the range under consideration, except the longest-wavelength edge. Besides, an increase in azimuth angle entails an increase in the shift of the TM with respect to TE efficiency maximum toward long wavelengths. Note also the largest spike in the –1 order TM efficiency near 46 Å, where the +1 order disappears, in which the relative efficiency is close to 1 and the absolute one is larger than 0.7. While an increase in rms roughness up to 20 Å brings about (see Fig. 13) a drop in reflection at the short-wavelength edge of the range which is smaller than that observed to occur at the 88° azimuth incidence angle, the values of the efficiency themselves are substantially higher. The proportional decrease in the efficiencies in all orders is about three times for 6 Å, 33% for 10 Å, and 16% for 15 Å.

The efficiencies obtained by modeling polygonal-profile gratings for azimuth incidence angles of 88 and 88.5° and an assumed rms roughness of 20 Å are listed in the table below for the wavelengths 9.98 Å and 13.34 Å to be compared with the results of measurements. One readily sees that the relative error of all the figures, with the exception of one, is not over a few tens of percents. The measured value specified in the table by asterisk[31] should apparently be considered unreliable. Although by using rigorous methods of efficiency analysis[8–10] and accurate means of groove profile measurement[18–20] one could achieve with an appropriate experimental accuracy a better agreement with the model[7,16–20], nevertheless, in this case it may be considered good. It should be taken into account that no precise data on the topology of the real gold profile, including its rms roughness, was available at the time of the calculation.

In conclusion to this Section, consider the results obtained in the modeling of optimal parameters and the final spectral response curves of the efficiency of gold-coated triangular gratings with 6000 gr/mm. Preliminary numerical modeling yielded optimal blaze angles for the –1 order and the wavelength of 15 Å for two azimuth incidence angles, 88 and 88.5°. They were found to be 7.65 and 10.3°, respectively. Figures 14 and 15 display the efficiency in the first three diffraction orders for the two incidence polarization planes calculated for gratings with these parameters and an rms roughness of 5 Å. As in the case of 5000-gr/mm gratings, the polar incidence angles were equal to the corresponding blaze angles. While the curves in Fig. 14 resemble very much those of Fig. 8, they exhibit a still stronger difference between the polarizations, because the grating has a shorter period and a larger depth. At the same time, the curves of Fig. 8 look preferable, particularly for the –3 order, whose efficiency at the maximum is twice higher. Of all the efficiency curves presented in this paper, those displayed in Fig. 15 for an incidence angle of 88.5° are the best. For instance, the efficiency in the –3 order near the maximum at 6 Å reaches 0.24 for the TE component and 0.31 for the TM, the efficiency in the –2 order near the maximum at the wavelength of 8 Å is 0.59 for the TE component and 0.65 for the TM, and the efficiency in the –1 order near the maximum at 15 Å is as high as 0.61 for the TE component, and 0.67 for the TM.

Table.

Wave length, Å	Azimuth incidence angle, 88°				Azimuth incidence angle, 88.5°			
	Absolute efficiency in a principal order		Sum of absolute efficiencies of orders		Absolute efficiency in a principal order		Sum of absolute efficiencies of orders	
	Modeling	Measuring	Modeling	Measuring	Modeling	Measuring	Modeling	Measuring
9.98	0.109	0.09	0.275	0.27	0.277	0.28	0.457	0.4
13.34	0.237	0.18	0.388	0.3	0.269	0.21	0.543	0.24*

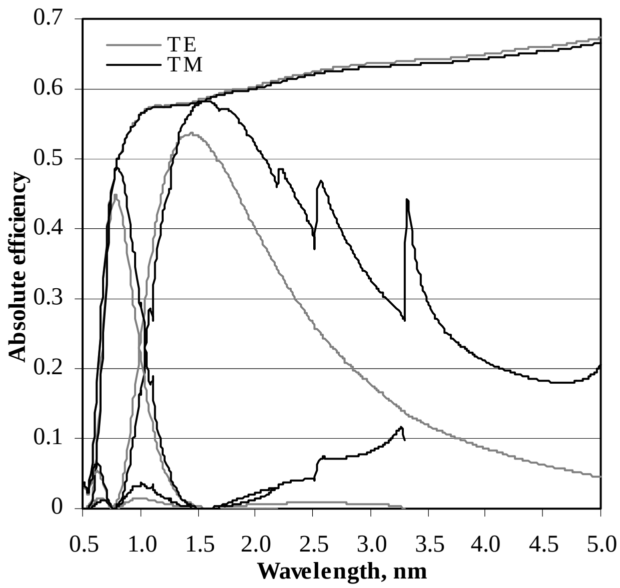

Fig. 14. Absolute efficiency in the –1, –2, and –3 orders of a 6000-gr/mm triangular grating with 7.65° working facet angle and 5-Å rms roughness calculated as a function of wavelength for the 7.65° polar and 88° azimuth incidence angles and the off-plane mounting.

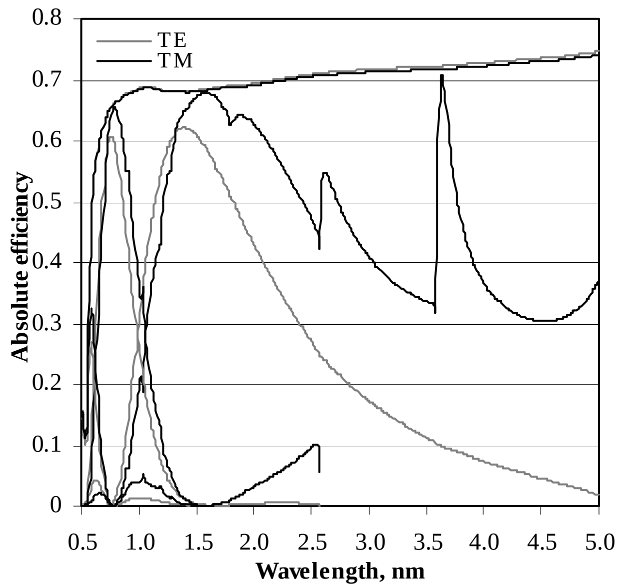

Fig. 15. Absolute efficiency in the –1, –2, and –3 orders of a 6000-gr/mm triangular grating with 10.3° working facet angle and 5-Å rms roughness calculated as a function of wavelength for the 10.3° polar and 88.5° azimuth incidence angles and the off-plane mounting.

5. CONCLUSION

In this paper, we have demonstrated the potential of the rigorous modified integral method and of the relevant PCGrate®-SX computer program for efficiency calculations of soft x-ray gratings intended for both the in- and off-plane diffraction mountings in the RGS. An efficiency analysis of gratings meeting the very high level of requirements for the SXT assigned for the Constellation-X mission shows the off-plane design to have considerable advantages over the in-plane arrangement. The best available low-frequency gratings acceptable for the RGS in-plane configuration cannot have an absolute efficiency in excess of 0.2–0.3 in the –1 order for both polarizations, while their maximum efficiency in the –2 and –3 orders is several times lower still. The maximum absolute efficiency for the off-plane RGS mounting may be as high as 0.7 for the TM component in the –1 order, and its average value is also a few times higher than that of the in-plane design throughout the range covered. The absolute efficiencies in the –2 and –3 orders in grazing off-plane diffraction geometries may reach very high values comparable to those obtained in the –1 order, which permits using the high orders in the shortest-wavelength part of the operating range to the maximum extent possible. To obtain high absolute efficiencies in the spectral region of interest, one should employ high-frequency gratings which have a depth (blaze angle) to period ratio large compared to the in-plane mountings and operate at the extreme grazing azimuth angle of incidence. Operation at a more grazing azimuth incidence angle (88.5 against 88°) has its advantages, because the absolute efficiencies in the shortest-wavelength part of the range increase, while the effect of roughness decreases. Gratings operating in the grazing off-plane diffraction regime are characterized by a strong manifestation of polarization effects and Rayleigh anomalies in the TM component, which requires invoking rigorous calculations. All the same, the average efficiency of an off-plane diffraction grating in unpolarized light exceeds by a factor 2–2.5 those obtained in an in-plane mounting.

As new and more precise data become available, we shall continue this study for both RGS mountings. We have not presented here efficiency calculations performed for real groove profiles because of the lacking AFM data. Besides providing information on the groove shape, AFM measurements permit one to determine the roughness, whose inclusion is necessary in precision modeling, by integrating the PSD function over the spatial frequency range. More detailed and precise efficiency measurements made, for instance, with synchrotron radiation, are also necessary. The present communication reports on several numerical calculations to find the optimal profile shape parameters and incidence angles based on maximization of the –1 order efficiency at a given wavelength. This optimization can be carried out for other wavelengths and other orders, as well as in an integral form for the whole range, using additional criteria.

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