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Diffraction Efficiency of Radially-Profiled Off-Plane Reflection Gratings

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ABSTRACT

Future X-ray missions will require gratings with high throughput and high spectral resolution. Blazed off-plane reflection gratings are capable of meeting these demands. A blazed grating profile optimizes grating efficiency, providing higher throughput to one side of zero-order on the arc of diffraction. This paper presents efficiency measurements made in the 0.3 – 1.5 keV energy band at the Physikalisch-Technische Bundesanstalt (PTB) BESSY II facility for three holographically-ruled gratings, two of which are blazed. Each blazed grating was tested in both the Littrow configuration and anti-Littrow configuration in order to test the alignment sensitivity of these gratings with regard to throughput. This paper outlines the procedure of the grating experiment performed at BESSY II and discuss the resulting efficiency measurements across various energies. Experimental results are generally consistent with theory and demonstrate that the blaze does increase throughput to one side of zero-order. However, the total efficiency of the non-blazed, sinusoidal grating is greater than that of the blazed gratings, which suggests that the method of manufacturing these blazed profiles fails to produce facets with the desired level of precision. Finally, evidence of a successful blaze implementation from first diffraction results of prototype blazed gratings produce via a new fabrication technique at the University of Iowa are presented.

Keywords: X-rays, X-ray diffraction, reflection gratings, off-plane, OGRE, blazed gratings, radial grooves

1. INTRODUCTION

Grazing-incidence diffraction gratings in the off-plane, or conical, mount can be used to perform high resolution, high throughput spectroscopy in the soft X-ray regime (~0.2–2.0 keV). This range contains a wealth of spectral lines, and an improvement in resolving power in this energy range will allow the characterization of important diagnostics of hot astrophysical plasmas. With theoretical resolving powers of $\lambda/\Delta\lambda = 5000$[1] and theoretical relative efficiencies approaching unity[2], radially-profiled reflection gratings with high groove densities in the extreme off-plane mount can offer more than an order of magnitude improvement in both resolution and effective area over current-generation observatories. This paper will focus on the efficiency of gratings fabricated as part of a grating study for the OGRE sounding rocket payload[3].

1.1 Off-Plane Grating Geometry

In the off-plane mount, light is incident on the gratings quasi-parallel to the groove direction and is diffracted into an arc along a cone of half angle γ. The diffraction equation, shown in figure 1, is then

$$\sin\alpha + \sin\beta = \frac{n\lambda}{d\sin\gamma}$$

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where α is the azimuthal angle to zero order along the cone with half-angle γ, β is the azimuthal angle corresponding to the diffracted order, and d is the groove spacing. The grooves can be radially-profiled, as demonstrated in the right side of figure 1, such that the groove spacing decreases along the optical axis and converges at the focal plane of the telescope. The radial groove profile provides a constant angle α across the grating and a constant β at the focal plane, minimizing any grating-induced aberration, which is necessary to maximize resolution. Additionally, the fact that the lines of interest are diffracted orthogonal to plane of the incident light allows for efficient packing geometry for an array of off-plane gratings.

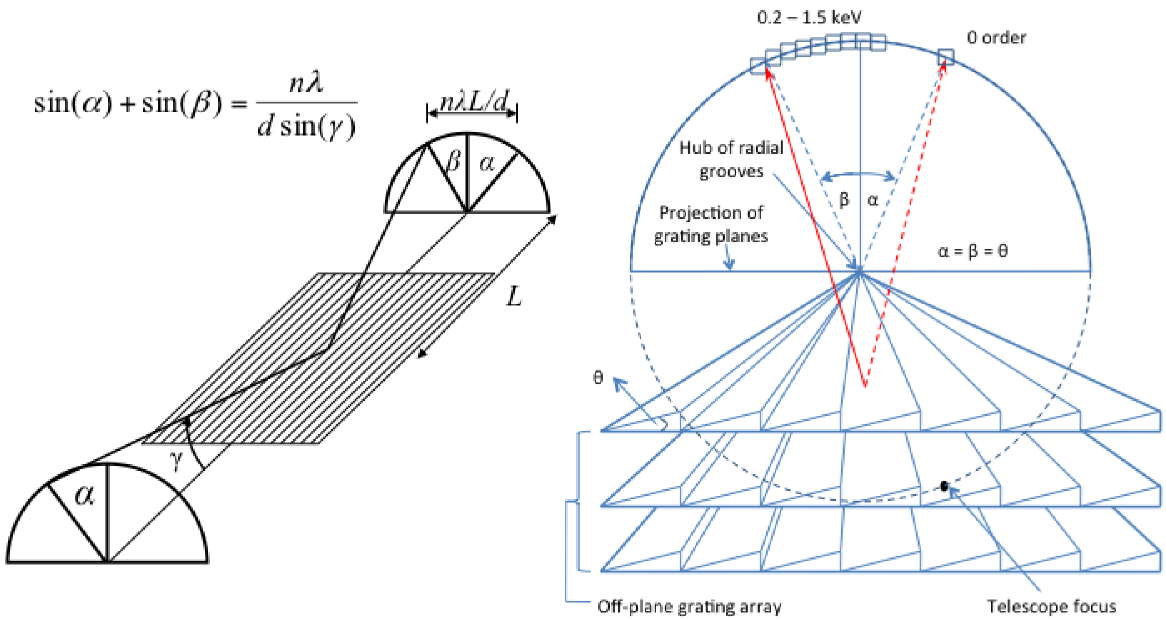

Figure 1: Geometry of the off-plane grating mount[4]

Off-plane reflection grating facets can also be blazed so that the grating preferentially diffracts incident light of a specific energy, enabling maximization of the efficiency in a particular band of interest. By aligning the grating relative to the incident beam such that $\alpha = \beta = \theta$ (known as the Littrow configuration), where θ is the angle of the blazed facets, the diffraction efficiency is maximized at the energy corresponding to the dispersion angle β. Specifying the blaze angle θ enables one to choose the wavelength at which efficiency is maximized, λ_b (referred to as the "blaze wavelength"), measured by

$$\lambda_b = \frac{2d\sin\gamma\sin\theta}{n}$$

1.2 Motivation

The gratings discussed in this paper are part of an ongoing study to determine the most suitable gratings for the Off-Plane Grating Rocket Experiment (OGRE) sounding rocket payload. The gratings are also analyzed in anticipation of the demands of future large-scale X-ray spectrometers. The first design objection in grating fabrication is to achieve high diffraction efficiency, which increases the instrument's effective area. For the current OGRE telescope design, the gratings will need to reach ~50% absolute efficiency to achieve the desired effective area[3]. The second major design goal is the grating's resolving power (OGRE's target resolving power is $\lambda/\Delta\lambda$ = ~2000). To achieve this resolution level, an accurate radial groove profile is necessary in order to limit grating-induced aberration. Achieving OGRE's performance requirements and successfully flying the OGRE grating arrays on a sounding rocket will serve as a proving ground for the technology readiness of the gratings pertaining to future missions.

2. BESSY II SYNCHROTRON EFFICIENCY MEASUREMENTS

A set of off-plane gratings were tested for efficiency across a range of soft X-ray energies at the PTB Bessy II synchrotron. The soft X-ray beamline at BESSY II incorporates a vacuum chamber that contains a sample goniometer which provides six degrees of freedom. The setup also features a detector arm with two additional degrees of freedom. The synchrotron radiation comes from a dipole bending magnet and is focused and dispersed, using a combination of mirrors and gratings, to produce a pencil X-ray beam of monochromatic light that is tunable between 50 eV and 1.9 keV[5].

2.1 Description of Gratings

Three gratings fabricated via photolithography were tested at PTB. These gratings were manufactured by Jobin Yvon (JY) to produce a final blazed grating with a high groove density (>4000 grooves/mm) and a radial groove profile. A sinusoidal master was tested for efficiency, as well as a blazed grating produced directly from the sinusoidal master. The third grating was fabricated independently of the sinusoidal master with a higher groove density. However, the holographic ruling technique used to implement the grooves was unable to radially rule a grating with such a high groove density, so the third grating has parallel grooves. Each grating tested at PTB was coated in a layer of platinum and measured 52 x 52 x 7 mm. The specifications of each grating are summarized in table 1.

Table 1. Grating specifications for holographic gratings tested at PTB.

Grating	Facets	Density	Groove Pattern
CV43D	sinusoidal	4245 grooves/mm	radial
U3787	9^o blaze	4245 grooves/mm	radial
U3731	16^o blaze	5870 grooves/mm	parallel

2.2 Results

The first experiment performed at PTB was to test the efficiency of each grating with $\alpha = 0$. Absolute efficiencies were measured from 300 eV to 1.5 keV in 50 eV steps for 0^{th} order and three orders on each side of 0^{th}. The second experiment puts grating U3787 (with a 9^o blaze) in Littrow configuration such that $\alpha = \beta = \delta = 9^o$. The same grating is also tested in the anti-Littrow configuration, where $\alpha = -\delta$. Measurements are provided from 300 eV to 1 keV for 0^{th} order and positive and negative first order and are compared to PCGrate models for an idealized grating profile. The third and final experiment performed at PTB put grating U3731 (16^o blaze) in Littrow and anti-Littrow configurations with measurements from 300 eV to 1 keV for 0^{th} and positive and negative first orders. Results are summarized in the following plots.

Experiment 1: $\alpha = 0$

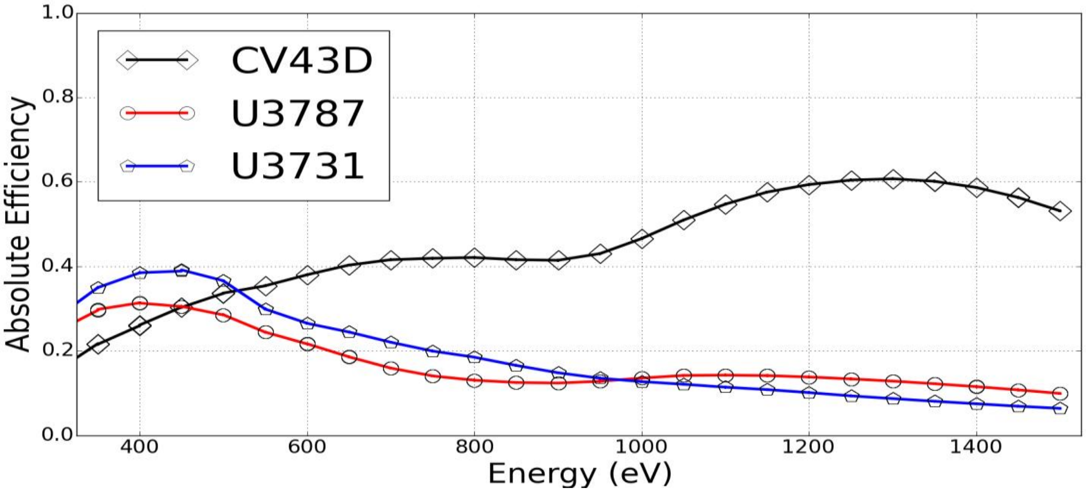

Figure 2: Total diffraction efficiency (three orders on each side of 0^{th}) for all three gratings.

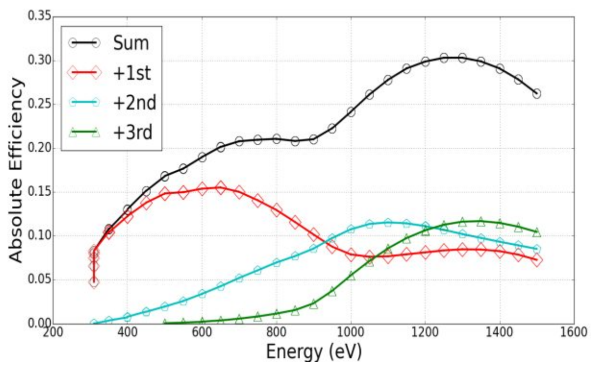

Figure 3a: CV43D positive orders

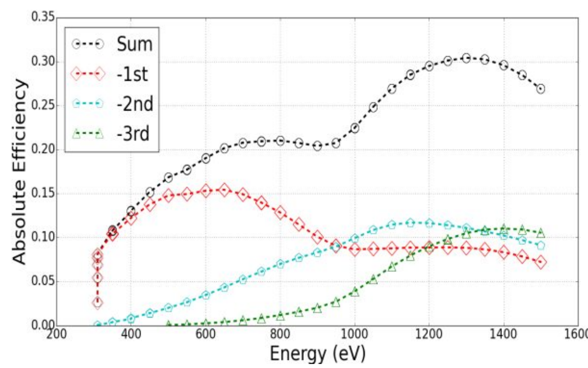

Figure 3b: CV43D negative orders

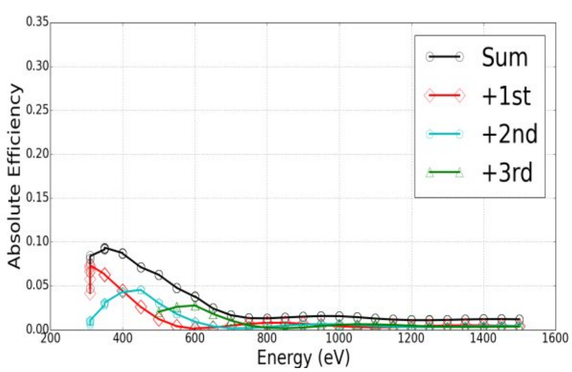

Figure 4a: U3787 (9^{o} blaze) positive orders

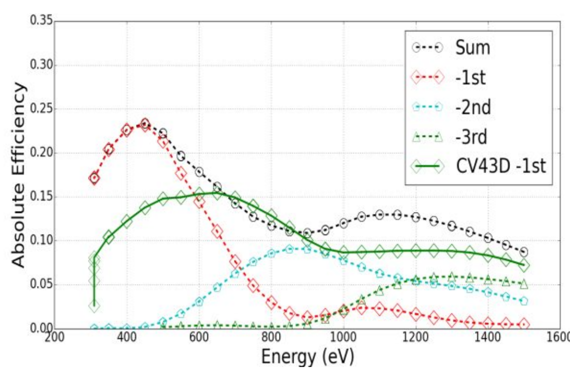

Figure 4b: U3787 (9^{o} blaze) negative orders

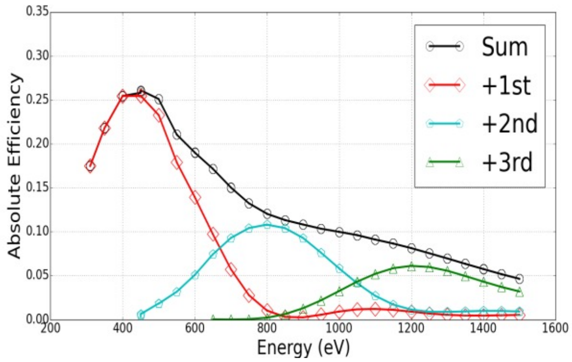

Figure 5a: U3731 (16º blaze) positive orders

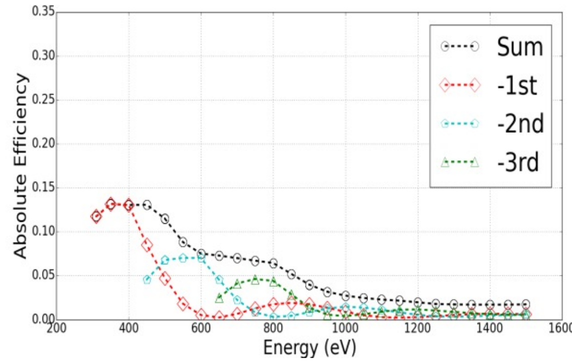

Figure 5b: U3731 (16º blaze) negative orders

Experiment 2: U3787 in Littrow and anti-Littrow compared to PCGrate model

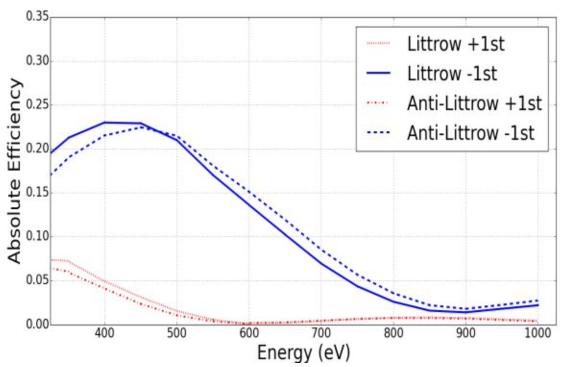

Figure 6a: U3787 (9º blaze) measurements

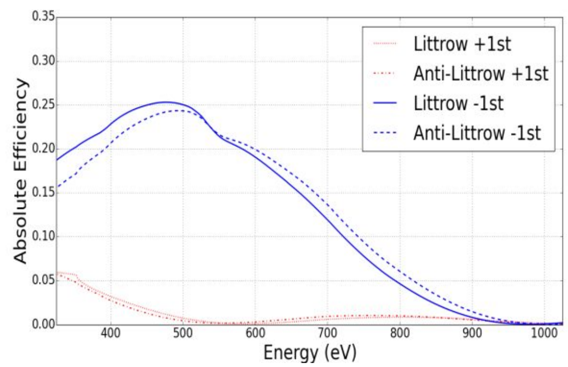

Figure 6b: U3787 (9º blaze) PCGrate models

Experiment 3: U3731 in Littrow and anti-Littrow compared to PCGrate model

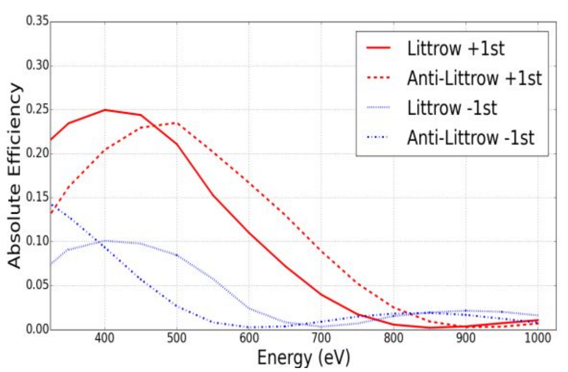

Figure 7a: U3731 (16º blaze) measurements

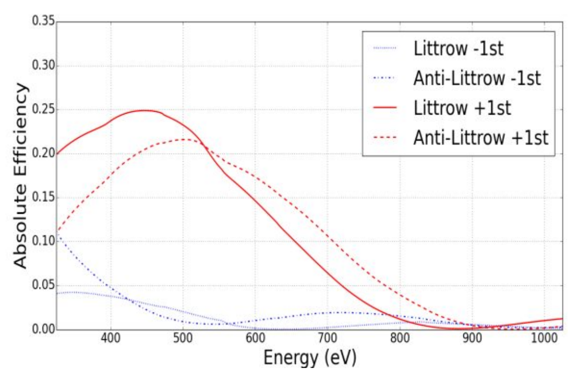

Figure 7b: U3731 (16º blaze) PCGrate models

2.3 Discussion

Absolute efficiency results from each grating demonstrate high diffraction efficiency. The sinusoidal grating (CV43D) shows equal efficiency on both sides of 0^{th} order, with no preferential diffraction. The total absolute diffraction efficiency of the sinusoidal grating exceeds 50% above ~1.1 keV, which meets OGRES's efficiency requirements. Testing both blazed gratings with $\alpha = 0$ (1^{st} experiment) provided evidence of a successful implementation of the blazed facets; each grating places the majority of diffracted flux into the side of zero order consistent with the blaze facets (negative for U3787 and positive for U3731). Figure 4b shows the negative orders of grating U3787 plotted with grating CV43D -1^{st} order. Since the absolute efficiency in -1^{st} order is higher for the blazed grating (U3787) than for the sinusoidal grating, we can determine that the blazed facets are effectively putting more diffracted light onto that side of zero order than the sinusoidal grating did.

Results of experiment two, which placed grating U3787 (9^{o} blaze) in Littrow and anti-Littrow configurations, show that throughput is optimized at -1^{st} order, consistent with expectations. We also see in figure 6a that the energy at which the grating's peak efficiency falls shifts slightly to higher energies, a feature that is also evident in the model shown in figure 6b. This could be due to the fact that as we shift to the anti-Littrow configuration, the blazed facets appear shallower to the incident beam, which will cause the X-rays to disperse closer to 0^{th} order – not as far out on the arc of diffraction. Since longer wavelength light is dispersed farther from 0^{th} order, shifting the diffraction closer to 0^{th} order corresponds to shorter wavelengths and higher energies, consistent with measurements and predictions. Similarly, experiment three (U3731 in Littrow and anti-Littrow) shows efficiency optimization in $+1^{st}$ order and the same characteristic peak efficiency shift to higher energies.

While the efficiency in -1^{st} order is higher for the U3787 grating than the sinusoidal CV43D grating, providing evidence that the blaze implementation successfully shifts efficiency into the wavelengths correlated with the blaze, results show that the total diffraction efficiency suffers significantly for the blazed grating compared to the sinusoidal grating (figure 2). Since grating U3787 is identical to CV43D with the exception of the blaze, this indicates that the implementation of the blazed facets negatively influences diffraction efficiency. In the photolithographic technique used to fabricate these gratings, the blazed facets are created with a directional ion etch, which likely produces rough groove facets that contribute to scatter (AFM analysis is currently being performed on the gratings, which will give us more insight into the surface features of each grating). Additionally, the photolithographic technique used to fabricate these gratings has failed to yield an ideal radial groove profile, which is crucial to meeting resolution requirements. Due to the imperfect blaze application and unsuccessful radial groove convergence with this fabrication technique, focus was shifted to other grating fabrication methods.

3. E-BEAM LITHOGRAPHY AND PRELMINARY RESULTS

In response to the need to improve upon blazed grating efficiency and resolving power, a team at the University of Iowa has developed an alternate grating fabrication method. This fabrication technique, which begins with a pre-master created using e-beam lithography, has already shown the ability to implement an accurate radial profile[6]. The gratings are fabricated with the following goals in mind: high groove density (>6000 grooves/mm), radial groove pattern, ~100 cm^2 grating area, and the ability to implement a variety of blaze angles without significantly altering the fabrication procedures[6,9].

3.1 Prototype Testing at MPE PANTER

A prototype grating created using this e-beam lithographic technique was tested at the Max Planck Institute for extraterrestrial Physics (MPE) PANTER X-ray facility. PANTER has a 120 meter long, 1 meter diameter beamline with a 12 x 3.5 meter test chamber. The grating tests performed at PANTER included a silicon pore optics (SPO) stack supplied by cosine Optics and a magnesium X-ray source. The primary purpose of this grating experiment was to perform alignment and resolution tests[7,8] for the OGRE sounding rocket and Arcus, a proposed SMEX mission, but the data collected does provide some insight into the grating's efficiency performance.

The grating tested at PANTER measured 25 x 32 x 0.7 mm (a factor of ~10 thinner than the gratings discussed above) and was imprinted onto a silicon wafer and etched to a 29.5^{o} blaze angle (this angle matches the desired blaze angle for

OGRE). The grating had an average groove density of 6033 grooves/mm and a radial profile converging over 8.5 meters (taking full advantage of the size of PANTER's test chamber and a reasonable baseline for SMEX-class missions). The grating was tested at a graze angle of 0.6°. In this alignment, the blaze wavelength discussed in section 1.1 is the +2nd order Mg-Kα line. This means we should expect the grating to preferentially diffract light to the positive side of zero-order, and specifically the +2nd order magnesium line.

Figure 8 shows the theoretical arc of diffraction for the grating place in its Littrow configuration, and table 2 shows some relative efficiency measurements with comparison to the photolithographic gratings discussed above. Figure 8 shows that the accessible orders in the PANTER test setup with the grating in Littrow configuration range from Mg-K -1st to Mg-K +2nd, which allows a direct comparison of the amount of incident light diffracted into those orders. We see that +1st order has a factor of about 40 times more light diffracted to it than does -1st order, and +2nd order (the line corresponding to our blaze wavelength) has another factor of ~2 more light than +1st. While these numbers do not provide insight into the grating's absolute efficiency, we do see strong effects of the blaze, as nearly all of the diffracted X-rays are on the positive side of zero order (the side corresponding to the blazed facets). This test delivered clear evidence of a blaze implemented at a specific angle (29.5°) on a grating with highly dense, radial grooves, fulfilling three of the four goals for this grating study. Additionally, evidence of the blaze effect has been shown on gratings with 10° and 54.7° blaze angles using this fabrication method[6,9], so we see that the fabrication processes are easily adapted to fit a variety of blaze angles.

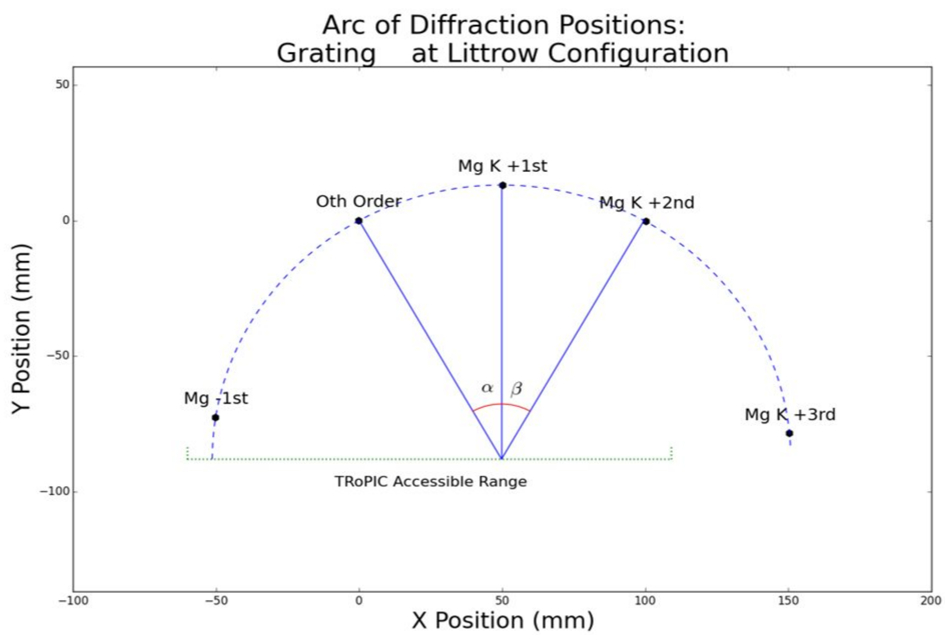

Figure 8: Diffraction orders accessible in Littrow configuration with PANTER detector TRoPIC

Table 2. Grating specifications for holographic gratings tested at PTB.

Grating	**U3787 (9° blaze)**	**U3731 (16° blaze)**	**PANTER - 29.5° blaze**	**PANTER - 29.5° blaze**
Orders Compared	-1st/+1st	+1st/-1st	+1st/-1st	+2nd/+1st
Relative Efficiency	4.7 ± 0.0	2.5 ± 0.0	43 ± 10	1.80 ± 0.04

In the coming months, the grating prototypes already produced will be independently tested for efficiency at the BESSY II synchrotron. The gratings will then need to be tested for resolution and, once efficiency and resolution requirements have been met, scaled up to sizes of ~ 100 sq. cm.

4. SUMMARY AND FUTURE WORK

As part of grating development for the OGRE sounding rocket and future X-ray spectrometers, various grating fabrication techniques were examined. Blazed gratings produced via photolithography were tested for efficiency at the BESSY II facility. Results indicate that the sinusoidal gratings fabricated with photolithography are capable of meeting efficiency requirements, but the sinusoidal efficiency is not retained when blazed facets are etched into the grating. Additionally, the necessary radial groove profile to achieve high spectral resolution was not achieved with this fabrication method. An alternative fabrication process focused on e-beam lithography has been developed at the University of Iowa. This method has produced thinner gratings with a higher groove density and an accurate radial profile. Early results indicate strong evidence for a successful blaze implementation for a variety of blaze angles. Follow-up tests will determine the gratings' diffraction efficiency and resolving power, and once mission parameters are met for these two items, large-format gratings will be produced and flown on the suborbital rocket payload OGRE to demonstrate the technology readiness of these gratings.

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