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ABSTRACT

An X-ray spectrograph consisting of aligned, radially ruled off-plane reflection gratings and silicon pore optics (SPO) was tested at the Max Planck Institute for extraterrestrial Physics PANTER X-ray test facility. The SPO is a test module for the proposed Arcus mission, which will also feature aligned off-plane reflection gratings. This test is the first time two off-plane gratings were actively aligned to each other and with a SPO to produce an overlapped spectrum. We report the performance of the complete spectrograph utilizing the aligned gratings module and plans for future development.

Keywords: Diffraction, gratings, grazing incidence, holography, x-rays

1. INTRODUCTION

Arcus 1 is a proposed X-ray spectrograph to be installed on the International Space Station. This spectrograph consists of silicon pore optics (SPO) 2 and blazed, radially ruled off-plane reflection gratings optimized for the feature-rich soft X-ray regime. The mission will utilize the SPO being developed for ESA’s Athena mission by cosine Research and reflection gratings being developed in collaboration between the University of Iowa and MIT/Lincoln Labs. The Arcus mission will answer key science questions related to structure formation in the Universe, supermassive black hole feedback, and stellar life cycles. To meet its science objectives, Arcus will have a resolution of λ/Δλ > 2500 and effective area > 600 cm² in the critical science bandpass around the O VII and O VIII lines (22.6 – 25 Å ). The mission will have a minimum resolution and effective area of λ/Δλ > 1300 and > 130 cm² over the entire bandpass (8 – 52 Å ) with λ/Δλ reaching ~3000 at the longest wavelengths.

Performance testing of aligned, off-plane reflection gratings with a SPO module was carried out at the PANTER 3 test facility of the Max Planck Institute for extraterrestrial Physics (MPE) in October 2014. During the test, two radially ruled, off-plane reflection gratings were was aligned to the SPO test module. The gratings used in this test were developed at the University of Iowa and are detailed in McEntaffer et al. (2013). This test was the first time that off-plane diffraction gratings were aligned with an SPO, and that two off-plane gratings were aligned to one another in situ to produce an overlapped spectrum. This paper describes the performance of the spectrograph composed of an SPO module and the aligned gratings module. To assess the contribution of the aligned gratings to the line spread function (LSF) of the spectrograph, the line widths of the SPO module alone and the first order Mg-K line of the complete spectrograph are compared. While not covered in depth here, comprehensive detail of the alignment methodology and results will be given in Allured et al. (In preparation). This paper is organized as follows: the components of the spectrograph are detailed in §2, a brief overview of the alignment procedure is given in §3, CCD image reduction steps and measured line widths are presented in §4, and discussion of the results in §5.

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2. SPECTROGRAPH ASSEMBLY

The spectrograph assembly tested at the PANTER facility consists of a SPO telescope, off-plane reflection gratings, and a CCD detector at the grating focal plane. A schematic of the SPO, grating, and focal plane positions within the test chamber is shown in Figure 1. An image of the components installed in the PANTER vacuum chamber during initial grating alignment with a laser is presented in Figure 2 where the SPO stack is closest to the camera and the grating module is visible in the background.

2.1 Silicon Pore Optics

SPO have been developed for the past 10 years by a consortium led by cosine Research, and have become the main technology for the X-ray mirror of the Athena mission. SPO make use of industry standard super polished silicon wafers. These wafers are first diced into mirrors plates of the desired rectangular shape. Then each plate is
wedged so that a focusing optics is formed when multiple plates are stacked onto a conical mandrel. Before being stacked, the plates are ribbed, leaving a thin membrane on one side used to reflect the X-rays, and a number of ribs on the other that are used to bond to the next plate. This results in pores in the SPO stack, through which the X-rays can reflect and travel to the focal plane detector. If necessary to meet science requirements, plates may also be coated to increase their reflectivity. An SPO stack is very stiff, light-weight, and the stacking process is such that the figure of the mandrel is reproduced with high fidelity so that by combining two stacks in a mirror module, a high resolution imaging system can be built.

For this campaign, a single SPO stack was built. The stack consists of 13 plates, with radii between 450 and 439 mm, width of 66 mm, and length along the optical axis of 22 mm. Its geometry approximates that of a parabolic reflector. With a focal length of 8 m, the wedge on each plate was tuned to deliver the required 10 arcsecond (") change in incidence angle between consecutive plates, resulting in a confocal system. For on-axis measurements, the incidence angle is of \( \sim 1.5^\circ \).

The SPO stack is shown in Figure 3 prior to installation in the PANTER vacuum chamber. Due to time and budget constraints, the SPO module for this test was shaped using a simple aluminum mandrel rather than one made of high quality polished fused silica. Therefore, it is important to note that the properties of this SPO module, while qualitatively similar to those in the planned Arcus design, are not characteristic of the state of the art in SPO manufacturing.

2.2 Gratings

A diagram of the off-plane grating geometry is shown in Figure 4. In the off-plane mount, light that is incident onto the gratings at a grazing angle and roughly parallel to the groove direction is diffracted into an arc. The diffraction equation for the off-plane mount is:

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

where \( \gamma \) is the polar angle of the incident X-rays defined from the groove axis at the point of impact, \( d \) is the line spacing of the grooves, \( \alpha \) represents the azimuthal angle along a cone with half-angle \( \gamma \), and \( \beta \) is the azimuthal angle of the diffracted light. The grooves are radially ruled such that the spacing between adjacent grooves decreases towards the focus to match the convergence of the telescope. The gratings tested at PANTER have
a laminar (rectangular) groove profile and average groove spacing of 6033 grooves/mm. The grating substrates are 100 × 100 × 0.7 mm Si wafers with a central grooved area of 25 × 32 mm.

For this test, two gratings were actively aligned together to demonstrate a technique for aligning nested diffraction gratings in an Active Alignment Module (AAM). The AAM consists of slots for the grating wafers and an exterior skeleton into which 5 picomotors are mounted in order to align sequential gratings to an initially installed fixed reference grating. The AAM is shown in Figure 5, where two of the five picomotors which are used to control grating yaw are visible on the top of the module and three motors are partially visible on the front of the module which control pitch and roll actuation of the active grating. For this test, only 1 additional grating was installed and aligned to the reference grating, though the procedure could be repeated to add more gratings as desired. The general installation and alignment procedure is as follows: a reference grating is bonded into the first wafer slot of the AAM. The active wafer is then installed into the adjacent wafer slot with springs between the active wafer and reference wafer surfaces and between the second wafer and the base of the AAM. Finally, the picomotor cage is installed and the 5 picomotors actuate to apply force against the active wafer which is balanced by the surface and base springs. The cage interface to the module is patterned to follow the spacing between gratings. One can now actuate the active grating and finely align it in situ using incident X-rays. The step size of each picomotor is approximately 30 nm, which translates to angular step sizes of ∼0.1″ in roll, pitch, and yaw. In the paper, the ‘active alignment module’ will refer to the entire module once the active grating was aligned with the reference grating, bonded into place, and the picomotors and springs disengaged.

2.3 Detectors

Three detectors were in use at the focal plane in the PANTER chamber during these test, TRoPIC, the ROSAT Position Sensitive Proportional Counter (PSPC), and PIXI. TRoPIC is a single photon counting detector with 75 μm pixels operated in frame-store mode. TRoPIC is a prototype of the eROSITA detector and is identical apart from its smaller pixel format of 256×256 compared to 384×384 and a lower operating temperature of approximately -100°C. The PANTER facility also has a spare of the ROSAT PSPC detector which we utilized for macro imaging of orders and for rough alignment due to its large active area (80 mm diameter) though relatively course spatial resolution of ∼250 μm. PIXI is a Peltier and water cooled Princeton Instruments PI-MTE-1300B integrating in-vacuum CCD with 20 μm pixels in a 1340×1300 format. All three detectors are shown in Figure 6. PSPC and TRoPIC are mounted onto the same translation stages and were able to image the 0 and ±1st orders. PIXI was mounted on a separate vertical translation stage sharing the other movements with TRoPIC and PSPC and was able to reach negative orders. This paper focuses on data obtained with the PIXI detector.
Figure 5: The AAM as viewed from the X-ray source direction. The top two picomotors control the active grating yaw while the three motors on the face of the grating (image right) actuate roll and pitch.

Figure 6: The X-ray detectors at the PANTER facility. From left to right: PIXI, TRoPIC, and PSPC.
3. PANTER TESTING

To investigate the performance of the spectrograph, the gratings and SPO were installed into the detector chamber of the PANTER test facility. The PANTER beamline consists of a multi-target electron impact X-ray source at the head of a 1 m diameter 120 m long vacuum chamber. The beamline ends in a 3.5 m by 12 m test chamber which easily accommodates the SPO, gratings, and detectors.

The gratings were mounted into the PANTER chamber within the AAM with 5 degrees of freedom relative to the SPO and CCD. In the coordinate space of Figure 1, the \( z \) position was set based on initial physical positioning and verified by laser distance measurement and linear translation stages in the \( x \) and \( y \) directions were used to position the grating module into the X-ray beam. A goniometer stage was used to control grating yaw, and a rotation stage controlled pitch. Roll alignment of the gratings was set via mechanical tolerance within the mount. All of the grating module stages were controllable outside of the vacuum chamber. The SPO light is incident on the gratings at an angle of 1.5\(^\circ\). This incidence angle was set using the separation between the SPO focus and the zeroth order reflection of an optical laser mounted at the head of the beamline and has an uncertainty of approximately 1 cm over the 8 m throw (\( \sim 4' \)). The chamber was then evacuated, and the PSPC was used find the various diffraction orders and to initially zero the reference grating yaw. A mosaic image of the diffraction orders taken by the PSPC detector is shown in Figure 7. In the mosaic, the active and reference grating are purposely offset in pitch to illustrate both gratings and the image is labeled with the various observable diffraction orders. We note that 3\( ^{\text{rd}} \) order Mg-K was also visible, though is not within the spacial extent of the PSPC mosaic. Rough alignment was accomplished with PSPC followed by fine alignment with PIXI and TRoPIC. The active grating was aligned to the reference grating by manipulating the AAM picomotors on the active grating (as discussed in §2). Once both gratings were aligned, the active grating was bonded in place, producing the aligned grating module of the spectrograph.

A narrow line is necessary to assess any focus broadening due to grating effects including misalignment. A naturally broad line would cause confusion with the spacial resolution of the telescope. Of the lines observed, Mg-K is the narrowest (\( \Delta E/E_{\text{peak}}=0.36 \text{ eV}/1254 \text{ eV} \)) compared to Cu-L (3.5 eV/930 eV), O-K (6 eV/525 eV) and Fe-L (3.5 eV/705 eV).\(^{11,12}\) Additionally, the best statistics were achieved in the 1\( ^{\text{st}} \) order Mg-K line compared with the lower count-rate, higher orders. Therefore, the spectrograph performance is characterized here based on the narrow 1\( ^{\text{st}} \) order Mg-K whose line width is representative of the spectrograph PSF in the dispersion direction.

4. REDUCTION AND RESOLUTION

This section outlines the reduction steps taken to extract LSF measurements from the CCD images taken at PANTER.

To process the raw PIXI images, a dark frame is first subtracted from the integrated image. The dark frame is a 1340\( \times \)1300 array whose pixels are the median value of \( N \) dark exposures taken consecutively. The dark frames are taken at the same position with the same exposure duration and close in time to the observation frames. The dark-corrected background is characterized by two background regions of the same size but spatially offset from the observation extraction region. The dark-corrected images are thresholded by setting to zero any pixels which fall below 3 times the background \( \sigma \) value. It is important to note that PIXI is not a photon counting detector and that the result of this processing is an image whose pixels represent (corrected) integrated analog-to-digital units (ADU).

The SPO focus is asymmetrical and is much wider in the non-dispersion direction compared to the dispersion direction. To calculate the dispersion direction LSF, the image is first collapsed in the non-dispersion direction. However, due to the asymmetrical shape of the focus, any misalignment with respect to the CCD \( x \) and \( y \) directions would skew the apparent LSF. Therefore, the image is initially rotated via a rotation matrix to account for any misalignment with the CCD. The applied rotation angle is found by performing a least squares fit of the form \( u = m v + b \), where \( u \) is in the dispersion direction, to the image weighted by each pixel value. Such a fit is illustrated in Figure 8. However, for lines with with few counts, the error on the least squared fit may be large, yielding a large error on the rotation to be applied. To better estimate the appropriate rotation, the CCD image is rotated through an array of angles and the fit is applied for each rotation, yielding a relationship between the measured slope and the applied rotation. An example of this procedure is shown in Figure 9, where
Figure 7: A mosaic image of the diffraction orders taken by the PSPC detector. The color scale indicates energy, which decreases in the dispersion direction from 0th order. The image is plotted in a log scale to bring out the individual lines, which are labeled on the right-hand side of the image. Third order Mg-K was also observed, though is not on the spatial scale of the mosaic.

Figure 8: Least squares fit of the form $u = mv + b$ (where $u$ is in the dispersion direction) applied to the image weighted by each pixel value. The fitted slopes are plotted versus an array of rotation angles. The best rotation is found as the intercept of this linear relationship where the fitted slope is 0, indicated in the plot by a dashed horizontal line.

Figure 10 shows the cropped and rotated PIXI image and projections of the SPO focus before grating installation. The point spread function (PSF) of a grazing incidence X-ray telescope is dominated by figure error and by scatter, with the scattering contribution being greatest in the in-plane reflection direction. For a full 360° optic, the PSF is circular with a bright, dense core surrounded by scatter dominated wings. The PSF can be be limited in a preferred direction by subaperturing the incident light, creating a focus which is narrow in the chosen direction. The effect of subaperturing for the test module is apparent in Figure 10 where the focus is much broader in the in-plane direction of the SPO contrasted with a narrow focus in the off-plane (grating dispersion) direction. The resolving power of the spectrograph is dominated by the extent of a line in

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the dispersion direction and is limited by the telescope focus in addition to aberrations added by the gratings.

The rotated CCD image is collapsed in the non-dispersion direction, and the resulting line width characterizes the LSF of the telescope. The SPO focus is not well described by a simple Gaussian model. Therefore, to avoid relying on an underlying distribution, the line width is described in this paper by the half-energy width (HEW) in the dispersion direction, where the HEW contains the central 50% of the line’s integrated counts as calculated from its cumulative distribution function (CDF). A Spline interpolation is applied to the CDF points allowing the HEW boundaries to fall between pixel values. The Spline interpolated CDF of the SPO focus is shown in Figure 11 where the vertical dash-dot lines indicate the upper and lower HEW bounds.

As noted above, PIXI is not a photon counting CCD and images are instead in units of integrated ADU without the availability of a direct conversion to photons. Because many ADU are created for each photon event, Poisson errors based on ADU significantly underestimate the percent error in each bin and subsequently on the HEW if calculated based on Poisson statistics. An error based on the assumption of Poisson statistics yields unrealistic uncertainty on the measured HEW of $\lesssim 0.1\%$. Instead, to estimate its uncertainty, the HEW is calculated individually in each of the sub-frames of the PIXI integration and the uncertainty taken as the standard deviation over these sub-frames. For the Mg-K PIXI integration presented here, this procedure is carried out with 19 sub-frames in the total integration. However, the SPO focus image contains only a single sub-frame, thus the uncertainty in the HEW cannot be estimated in the same manner and an uncertainty is not quoted. In order to most directly compare with the single long integration of the SPO focus, the HEW of the Mg-K line is measured from the summed image over all of the 19 sub-frames.

Figure 12 shows the width of the processed SPO focus in the grating dispersion direction (dashed line) overplotted with the first order Mg-K line (solid line) representing the overall spectrograph focus. The structure of both focuses appears similar, and the HEW of the SPO focus is found to be 2.31$''$ while the HEW of the Mg-K line is found to be 1.98±0.07$''$.

5. DISCUSSION

As a proof of methodology, we have demonstrated a spectrograph composed of silicon pore optics (SPO) and an aligned off-plane reflection grating module at the PANTER test facility. The point spread function (PSF) of the
Figure 10: The SPO focus imaged with PIXI is shown with projections in the dispersion and non-dispersion directions.
Figure 11: Spline interpolated CDF of the SPO focus. Units on the left y-axis are normalized to the sum of the line counts while units on the right axis are in ADU. Vertical dash-dot lines indicate the upper and lower bounds of the HEW.

Figure 12: Mg-K 1st order PIXI line profile (solid curve) overplotted with the SPO focus line profile (dashed curve). The HEW are found to be 2.31 and 1.98 ±0.07″ for the SPO and Mg-K lines, respectively.
spectrograph assembly is characterized by the half energy width (HEW) of the 1st order Mg-K line. The HEW of the SPO module is measured to be 2.31" in the dispersion direction while the HEW of the spectrograph is measured to be 1.98±0.07". The overall spectrograph line width is therefore found to be narrower than that of the SPO. A narrower line width for the spectrograph focus could be attributed to the grating module subaperturing the light from the SPO in the radial direction. While the SPO focus is an integration over all 13 of the SPO plates, the unmasked regions of the gratings only intercept light from approximately 2 SPO plates. Thus, any stack error contributions in the SPO will have a larger impact on the width of the SPO focus than on the final spectrograph focus.

We conclude that the current performance of the spectrograph is not limited by contributions from the aligned grating module and that the overall PSF is presently dominated by contributions of the SPO module. The SPO module focus extent in the dispersion direction is highly dependent on the figure of the SPO plates. Thus, improved performance can be achieved by reducing figure error in the optic. The quality of the forming mandrel is critical to the figure of the final optic. The current SPO test module plates were shaped using a simple aluminum mandrel due to time and budget constraints. In the future, figure quality of the SPO modules will be improved through the use of high quality polished fused silica mandrels which have previously been demonstrated by cosmic Research to produce optics with superior figure. These improvements may push into the regime of grating module contribution to the spectrograph focus.

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