Off-plane reflection gratings for Constellation-X

Randall L. McEntaffer[1,*], Webster Cash[2], & Ann Shipley[2]

[1]Department of Physics and Astronomy, University of Iowa, Van Allen Hall, Iowa City, IA 52242
[2]University of Colorado, Center for Astrophysics and Space Astronomy, Boulder, CO 80303

ABSTRACT

We present the latest design of an off-plane reflection grating array for the Constellation-X X-ray Grating Spectrometer. The off-plane design can easily demonstrate the baseline requirements of resolution, R > 1250 and throughput, effective area > 1000 cm^2 from 0.3 – 1.0 keV. Furthermore, the flexibility of the design allows for several avenues for optimization of these factors. We consider two configurations, 3 m and 9 m from the focal plane using a 20 m focal length telescope. The trade-offs between the two options are discussed.

Keywords: Constellation-X, off-plane reflection gratings

1. INTRODUCTION

1.1 Constellation-X

Constellation-X is the next large X-ray observatory combining large collecting area with high resolution spectroscopy over a broad range of X-ray wavelengths. Two main instruments provide the bandpass in the soft X-rays. First, the X-ray Microcalorimeter Spectrometer (XMS) collects light at the telescope focus and provides imaging and spectroscopy from 0.6 – 10.0 keV. Second, the X-ray Grating Spectrometer (XGS), diffracts light onto a CCD array and allows for high spectral resolution from 0.3 – 1.0 keV. In this lower energy range there are many fundamental plasma diagnostics such as the He-like triplet of astrophysically abundant elements, and absorption lines from active galactic nuclei outflows and warm-hot ionized medium (WHIM) filaments. These detailed line spectra and complex absorption line profiles drive the spectral resolution requirement of R > 1250 (E/ΔE) between 0.3 – 1.0 keV in order to obtain unambiguous physical constraints on these objects. Furthermore, these science objectives also require an effective area of more than 1000 cm^2 in this waveband, which is more than an order of magnitude increase compared to current X-ray observatories. However, there are a limited number of techniques that will support these requirements. Reflection gratings in the extreme off-plane mount are one of these techniques and offer a straightforward approach.

1.2 Off-plane reflection gratings

The off-plane mount at grazing incidence brings light onto the grating at a low graze angle, quasi-parallel to the direction of the grooves. The light is then diffracted through an arc, forming a cone, so that this mount is also known as conical diffraction[1,2]. The off-plane grating equation is

$$\sin\alpha + \sin\beta = \frac{n\lambda}{d\sin\gamma}, \tag{1}$$

where d is the spacing between grooves and γ is the angle between the direction of the incoming ray and the direction of the groove at the point of impact. Light comes into the grating at an azimuthal angle of α along a cone with half-angle γ. It is then diffracted along the same cone of half-angle γ, but now with an azimuthal angle of β. If γ is kept small (< 3°) then the arc of diffraction stays close to the plane of the grating. However, at these low angles even large gratings have a small cross section to the incoming light. The solution is to stack gratings in an array to intersect the desired amount of the telescope beam[3].

Using the grating equation shows that the spectral resolution of diffraction gratings can be expressed as

$$R = \frac{E}{\delta E} = \frac{\lambda}{\delta\lambda} = \frac{L\sin\gamma(\sin\alpha + \sin\beta)}{FB\cos\alpha}, \tag{2}$$

where B is the telescope resolution in radians and L/F is the ratio between the distance from the gratings to the focal plane (L, the throw) and the focal length of the telescope (F). This equation can be further simplified by considering a

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method for increasing the throughput for reflection gratings. The grating facets can be cut to emphasize a specific reflection geometry (referred to as a blazed profile) and therefore a specific β (or λ). The maximum efficiency occurs at a β that is equal to the incoming azimuthal angle, α, which is equal to the blaze angle on the grating. In this case the resolution equation can be simplified to

$$R = \frac{L 2\theta \tan\alpha}{FB}, \tag{3}$$

where θ is the graze angle and approximately equal to γ in the off-plane mount. This equation elucidates several avenues for increasing spectral resolution. For instance, working with a higher blaze angle, and therefore higher α and β, can increase the resolution dramatically. Doubling the blaze angle from 30° to 60° increases the resolution by a factor of 3. However, such high graze angles are currently difficult to fabricate. Therefore, the industry state-of-the-art will determine this factor. Second, increasing the graze angle linearly increases the resolution. However, reflection efficiency will decrease and throughput will suffer. In this case the balance between resolution and telescope coverage will need to be considered before a final design is determined. The two factors left to consider are the telescope resolution and the ratio between the throw and the focal length.

Although the telescope resolution is a number determined by the quality of the telescope, a technique known as subaperturing can be used to decrease the effective blur of the telescope and increase spectral resolution[4]. By only intersecting a fraction of the telescope beam (typically a pie shaped wedge) only a fraction of the telescope blur is sampled. In practice this can easily increase the resolution by a factor of four. Next, when considering the ratio L/F the closer the gratings are to the optic the closer this ratio is to one, thus maximizing the resolution. The downside to this is that the grating array needs to increase in size as it moves closer to the optics, thus increasing mass. A final technique to mention, which is not evident from equation 3, is the use of radial groove gratings[5]. Such gratings have a groove spacing that varies along the length of the groove so that they exhibit a convergence that matches the convergence of the telescope beam. In this way α is kept constant along the width of the grating, thus limiting the aberrations apparent in typical parallel groove gratings. The following designs utilize these techniques to produce a feasible spectrometer for Constellation-X that meets the performance requirements, would be easy to fabricate and has reasonable tolerances.

2. REFLECTION GRATING SPECTROMETER

2.1 Overview

In order to obtain high quality spectra with modest observation times, Constellation-X requires a large collecting area. One method through which this could be attained is a 20 m focal length telescope that is 3.4 m in diameter providing ~6 m^2 of collecting area and 5″ resolution. The Reflection Grating Spectrometer (RGS) presented here is designed to match this 20 m configuration, which is currently being studied for Constellation-X. Figure 1 shows the spacecraft configuration that is being considered. On the right side of this figure the spacecraft is compressed into an Atlas V fairing. When fully extended the spacecraft consists of the mirror assembly on one end, which is connected to an avionics bus module via a fixed conical metering structure, while on the other end the bench housing the detectors is extended via deployable masts 9 m away from the avionics bus. This paper considers two options for the placement of the RGS: 1) mounted on the avionics bus 9 m from the focal plane or 2) extended 3 m from the focal plane on an independent structure. The following sections will cover the gratings and modules that constitute the RGS, the 3 m configuration, the 9 m configuration, and a discussion of the trade-offs between them.

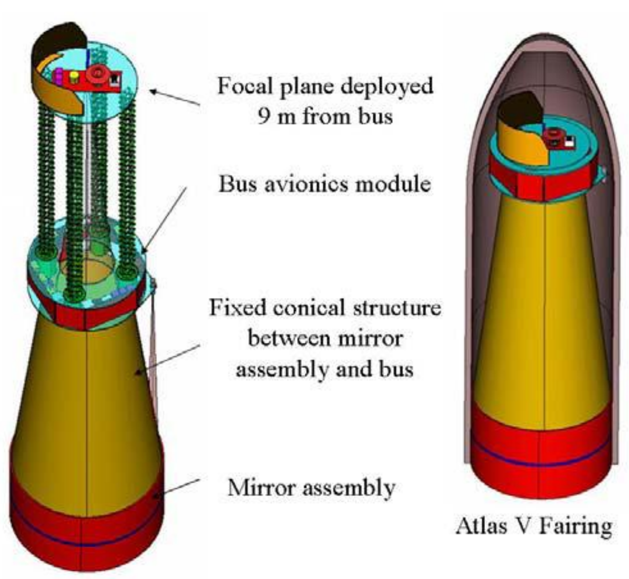

Figure 1: Monolithic 20 m focal length telescope design.

2.2 The RGS

2.2.1 The gratings

An example of an off-plane grating that can be used for these designs is displayed in figure 2. This grating measures 100 mm in the groove direction and 110 mm in the dispersion direction. These dimensions are not critical and can be tweaked to accommodate various configurations. An exaggerated radial groove profile has been sketched on the grating face for illustrative purposes. The groove density is 5500 g/mm with a blaze angle of 30°. Both of these factors are necessary to obtain R = 1250 for the 3 m configuration, but can be relaxed somewhat in the 9 m case. The substrates are trapezoidal with an edge thickness of 2 mm and a maximum thickness of 4 mm. If constructed from T6-6061 Al, these would weigh 0.09 kg each.

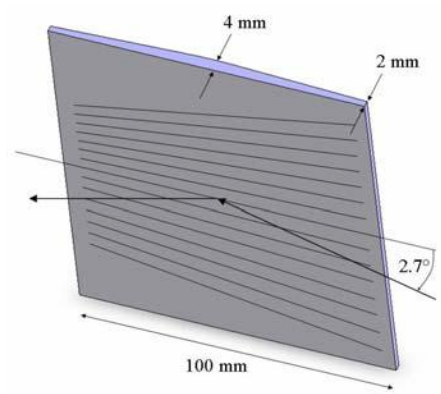

Figure 2: A single off-plane grating.

2.2.2 The grating module

Figure 3 shows a design for a prototype module of 18 of the above gratings. This module mounts the gratings near their center where the substrate is thickest. It is this structure that will maintain grating-to-grating alignment[5]. The gratings are fanned to maintain a graze angle of 2.7 degrees across the telescope beam. In both designs presented below the layouts show the modules placed along the Y-axis, but the placement of these modules is independent on azimuth. As these modules rotate around the Z-axis the CCD array will rotate an equal amount thus providing flexibility to the azimuthal placement of the CCDs on the focal plane. Furthermore, the graze angle on the gratings can be used to adjust the distance between the CCDs and the telescope focus; larger graze angles place the CCDs further from the telescope focus. However, there's a balance between graze angle, throughput, resolution and CCD array placement. For instance, larger graze angles provide lower throughput at higher energies and possibly an additional CCD in the array, but also provides higher resolution and possibly a more favorable configuration at the focal plane. The mass of one of these modules is ~ 2 kg.

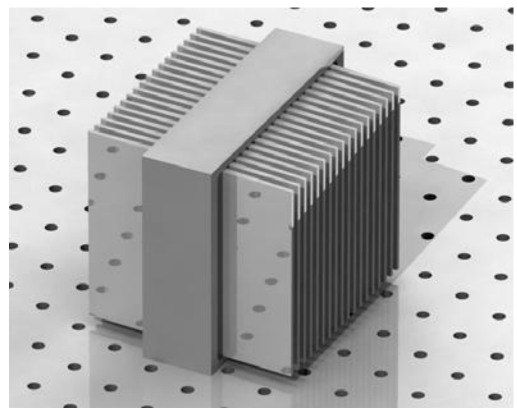

Figure 3: 18 gratings mounted into a module.

2.2.3 The 3 m configuration

Before the design of the two configurations is discussed the telescope layout needs to be considered. The telescope is a Wolter Type I with nested parabola primary mirrors and hyperbola secondary mirrors. The telescope node is at the intersection of the primary and secondary and measures 1.7 m on the outer diameter with a 0.372 m inner diameter. There are 376 active nested shells with a total geometric collecting area of 59,663 cm^2. The effective area of these shells is 34,332 cm^2 at 0.3 keV and 33,052 cm^2 at 1.0 keV. At 3 m from the focal plane the aperture area is condensed to 2.2% of that at 20 m. Therefore, in order to obtain the requirement of 1000 cm^2 the 3 m configuration grating array needs to cover 145 cm^2 at 28% total efficiency. This 28% level is obtained

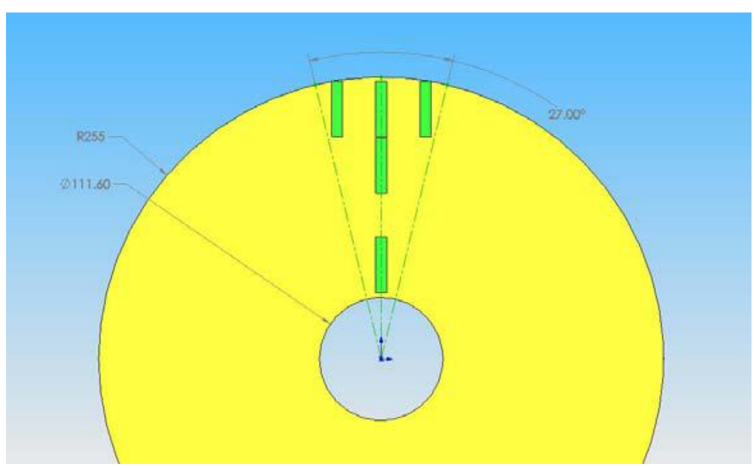

Figure 4: Telescope beam size at 3 m from the focal plane. The green lines depict the coverage area of the grating array. The green rectangles outline modules that were used for the ravtrace.

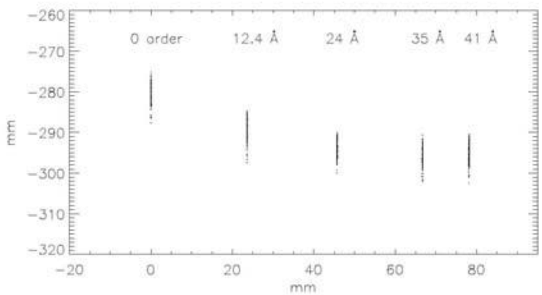

Figure 5: Spectrum resulting from the 3 m raytrace

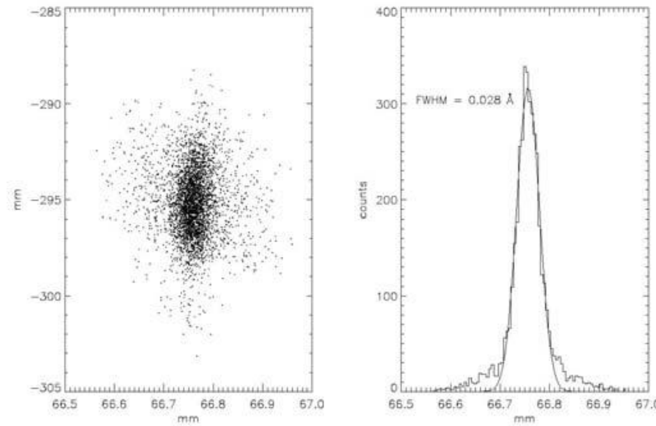

Figure 6: Left – spot diagram at 35 Å, right – histogram displaying R = 1250

from assuming 70% mechanical throughput and 40% absolute grating efficiency[6]. The required 145 cm^2 coverage translates to filling a pie wedge measuring 27° in azimuth. Figure 4 shows the telescope beam size at 3 m (yellow annulus) along with the 27° wedge outlined by the dark green dash-dotted lines. The green rectangles signify separate grating modules that were used to verify the design via raytrace. Each module measures 10 mm in the dispersion direction, 100 mm long in the groove and 50 mm in the array direction. In actuality the entire wedge should be filled with green rectangles, but only those shown were used in the raytrace since they signify the limits of the wedge and therefore the limits of the design. Previous raytrace verifications have been done for other Constellation-X configurations, but are not discussed here[7]. The results of the current design are shown in figures 5 and 6. Figure 5 shows the resulting spectrum at 0 order and wavelengths ranging from 1.0 keV to 0.3 keV. The left of figure 6 is the spot diagram at 35 Å for the combined modules shown in figure 4 and the histogram to the right has a full width at half maximum (FWHM) of 0.028 Å which results in a resolution of 1250 (λ/Δλ).

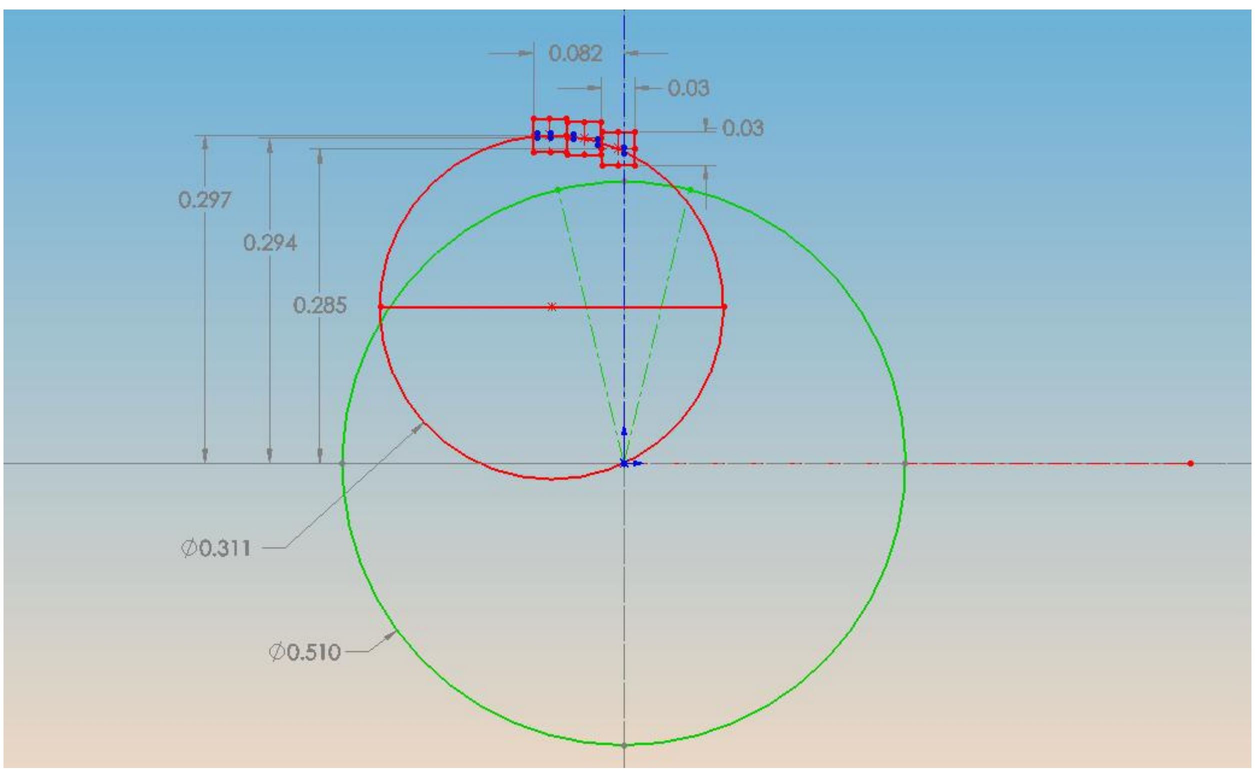

Figure 7: 3 m focal plane layout. The red circle is the arc of diffraction along which lie the CCDs (red squares). The green circle is the telescope outer envelope at 3 m from the focal plane with the telescope focus at the center.

The next design factor to consider is the CCD arrangement on the detector bench. Both designs assume 30 mm × 30 mm CCDs with 15 micron pixels. A telescope resolution of 5″ for a 20 m focal length telescope gives ~0.5 mm spot size on the CCD for 5′ FOV per 30 mm CCD. The focal plane layout is shown in figure 7. The green circle is the telescope beam outer envelope at 3 m and the center of this circle is the telescope focus. The green dash-dot line is the extent of the grating array again. The red circle defines the arc of diffraction for this off-plane configuration. The center of the red circle is the hub of the radial grooves on the gratings while the horizontal line is the projection of the gratings onto the focal plane. The red squares denote the position of the 3 CCDs required in this design to cover the bandpass. The need for only 3 CCDs is not only compact, simple and cost effective, but also saves considerable mass. The blue spots on the CCD show the positions of 0 order, 12.4 Å, 24 Å, 35 Å, and 41 Å from right to left.

The 3 m design exhibits a simple configuration consisting of a series of grating modules with gratings measuring 10 mm × 100 mm and filling 7.5% of the beam, thus keeping the overall size quite small. In fact, the total mass of gratings is less than 2 kg while the mounts should not add more than a few additional kilos. The array will need to be extracted from the beam during calorimeter usage and to limit scatter due to the structure; this will require some additional mass. Furthermore, in the case of the 3 m configuration an independent structure is extended from the focal plane to support the grating array in between the avionics bus and the detector bench. Northrop Grumman Space Technology (NGST) has done preliminary engineering of these two structures and suggest that the array could be rotated out of the beam via a flip mechanism with launch locks. Also, they conclude that the flip mechanisms combined with the support structure should weigh < 10 kg based on an existing design developed for the James Webb Space Telescope. This results in a total mass of < 15 kg for a mounted, actuated grating array. Therefore, the 3 m configuration consists of a compact, lightweight, simple design that meets the requirements for throughput and resolution.

2.2.4 The 9 m configuration

The 9 m configuration is similar, but scaled up to cover 9 times the area. Figure 8 shows the telescope beam envelope (yellow) at 9 m from the focal plane. Again, the green area consists of the modules used to perform the raytrace. In this case the modules are typically identical to those discussed in §2.2.2 and measure between 110 mm to 240 mm in the dispersion dimension. The total mass of a grating array that fills the entire required area plus structure is < 40 kg (10 kg for structure, 28 kg for gratings and mounts).

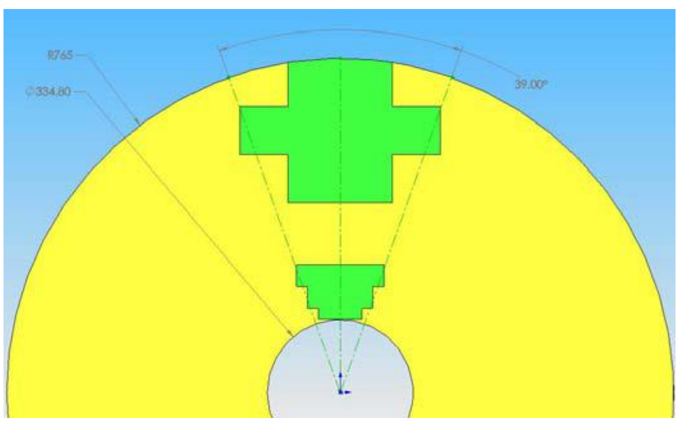

Figure 8: Telescope beam coverage at 9 m. The green area signifies the area used for the raytace.

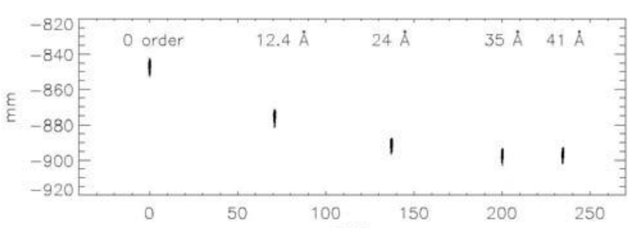

Figure 9: Raytrace of the 9 m design.

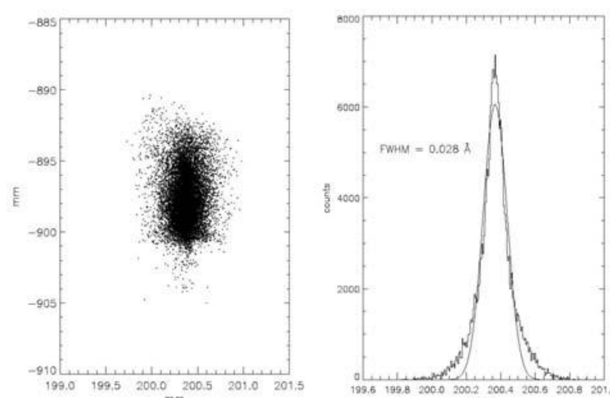

Figure 10: Left – spot diagram at 35 Å, right – R = 1250 (λ/Δλ)

The spectrum resulting from the raytrace is shown in figure 9. As expected, the wavelengths are dispersed three times as much as in the 3 m case, thus providing potential for more resolution. For this study modules were constructed and placed in the telescope only to reproduce the mission requirements. The spot diagram at 35 Å is shown in figure 10 and displays a resolution of 1250 (λ/Δλ). Finally, the CCD layout is shown in figure 11. Again, the telescope beam outer envelope at 9 m is outlined by the green circle. The center of this circle is the telescope focus. The dash-dot green lines are the coverage area for the grating array while the red circle is the arc of diffraction for the gratings. The red squares denote the positions of the seven 30 mm × 30 mm CCDs required to cover the bandpass. Since this design has three times the dispersion of the 3 m design one would expect a requirement of three times the CCDs. However, the area between zero order and 1.0 keV does not need to be covered thus reducing the number of CCDs required.

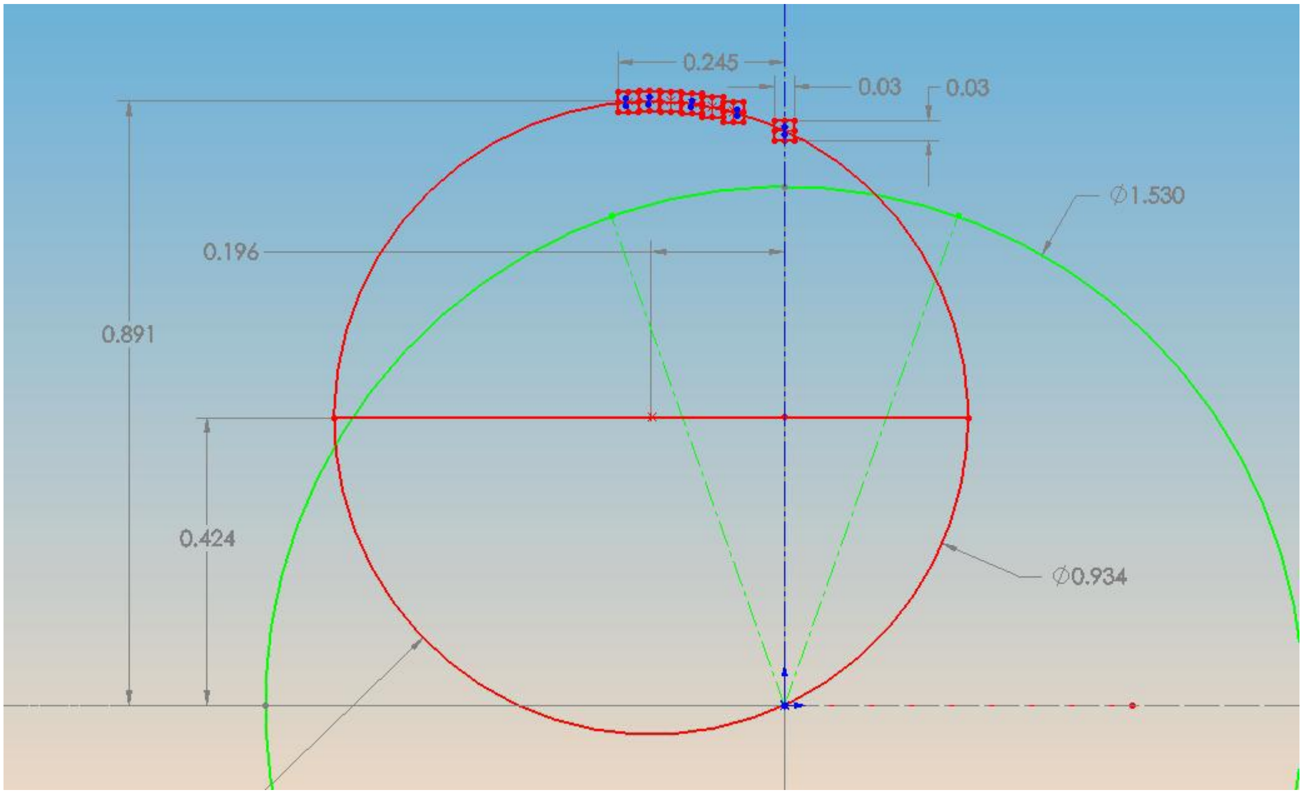

Figure 11: 9 m focal plane layout. Conventions are the same as in figure 7.

It is important to note that the resolution can be driven higher through optimization of every module. For instance, the cross dispersion width of the gratings can be reduced to take further advantage of subaperturing. Also, module attitude can be further manipulated to maximize spectral overlap at the focal plane. Other optimizations include varying the groove profile on each grating (where necessary) to limit aberrations, and slight displacements or rotations of the module to compensate for disparate path length distances. As seen in previous Constellation-X raytraces[7], one can also divide the wedge into 3 or 5 subwedges so that each subwedge samples an even smaller fraction of the telescope blur function. If the spectral lines from each subwedge were overlapped at the focus then this would gain no advantage. However, the contributions from each can be spread out in the cross dispersion direction to form a C shape that has as much resolution as a single subwedge. The cost/benefit analysis of pushing for high resolution is not the purpose of this paper, but will be continuously studied in depth during the development of the off-plane RGS.

2.2.5 Tolerances

The 6-axis module placement tolerances were calculated to maintain 1′ knowledge on the position of the zero order spot assuming that the grating-to-grating tolerances within the module are being maintained. These grating-to-grating tolerances are summarized elsewhere[5] and are not covered here. There are also module-to-module tolerances to consider, but these will be closer to the grating-to-grating tolerances than the tolerances stated here. For these tolerances the origin is considered to be at the center of a grating module cube and the axis orientation will be the same as that seen in figure 4, 7, 8 and 11: the X-axis is horizontal, the Y-axis is vertical and the Z-axis points out of the page. Table 1 lists the tolerances along with an explanation of their effect on the spectrum.

	3 m	9 m	Notes
δx	±3 mm	±3 mm	Moves the hub of the gratings by this amount and therefore moves the position of zero order by ± 3 mm on the detector, which is ± 30″.
δy	±3 mm	±3 mm	Moves the hub of the gratings by this amount and therefore moves the position of zero order by ± 3 mm on the detector, which is ± 30″.
δz	±30 mm	±90 mm	The projection of the hub and plane of the gratings upon the focal plane does not change but the throw of the gratings does, thus the radius of the arc changes as well. The throw effects the dispersion of the system and therefore affects the resolution. This tolerance is quite loose in comparison to x and y and may be as much as ± 100 mm, but 1% of the throw is conservative.
θx	± 3.4′	± 1.1′	Grating module pitch. Again, moves the position of the arc of diffraction. Scales with throw.
θy	± 6.7′	± 2.3′	Grating module yaw. This angle effects the position of the arc of diffraction at long wavelength more strongly than it effects the position of zero order. Therefore, this tolerance keeps 41 Å to within ± 1′. Scales with throw.
θz	± 15′	± 5′	Grating module roll. Moves zero order. Scales with throw.

Table 1: Grating array 6-axis position tolerances for the 3 m and 9 m configurations.

As evident from table 1, the tolerances are quite loose for the position of the entire grating array relative to a fixed telescope and focal plane. A fixed metering structure between the focal plane and the grating array in the 3 m configuration should supply ample support to meet these tolerances. For the 9 m case the tolerances are tighter, but should still be easy to meet given that they are mounted to the avionics bus which is directly tied into the optics via its own fixed metering structure. Once fixed to this structure, further knowledge of the array position can be gained from the telescope focus monitor.

Given the flexibility of the array placement tolerances, the tightest tolerances to consider will be the grating surface tolerances[5]. Optical surface errors can be introduced by a thermal gradient across the substrate. Due to this effect, we have run some basic thermal models and have come up with the following allowable thermal variations over a single grating (table 2). A more in depth discussion of the derivation of these can be found in Shipley & McEntaffer (2008, these proceedings). The temperature tolerances were calculated so that the resolution requirement (R = 1250) would be maintained.

Case	3 m (deg C)	9 m (deg C)
Allowable temp gradient along groove direction:		
Pitch direction (along grooves)	0.4	0.1
Roll direction (perp to grooves)	1.5	0.5
Allowable bulk temp change:		
Pitch direction (along grooves)	1.4	0.5
Roll direction (perp to grooves)	49.5	16.8

Table 2 : Allowable thermal variations over a grating for the 3 m and 9 m configurations to maintain R = 1250.

As expected, these tolerances scale with throw as well. Again, the 9 m case may benefit from the fact that the grating modules are attached to the fixed metering structure and not extended off the focal plane; the temperature control for the optics may be extended to the gratings. In the 3 m case the independent structure may need to either tie into the focal plane temperature control or incorporate its own thermal control depending on how well the focal plane is controlled and how severe the gradient will be in between the detector bench and the avionics bus. These tolerances depend strongly on how the grating is held and how much the mount and support structure is allowed to move with them. Our simple case assumes a constant gradient at all times and doesn't account for relaxing due to the structure moving as well (the mounting constraints are fixed in the model). Therefore, these numbers should be quite conservative[8]. Surface errors will be considerably reduced using an athermal mount design that removes mounting stress.

SUMMARY

Constellation-X is the next large X-ray telescope and as such requires large effective area and high spectral resolution. For soft X-ray energies this can be obtained in a straightforward manner using an off-plane reflection grating spectrometer. Two designs have been presented to elucidate two options: attaching the grating array 9 m away from the focal plane to an avionics bus that is hard-mounted to a 20 m focal length telescope, or mounting the grating array 3 m off of the focal plane using an independent structure. Both designs have been theoretically shown to meet the effective area requirement of 1000 cm^2 and resolution requirement of 1250 ($\lambda/\Delta\lambda$). Also, the tolerances on the position of the grating arrays within the spacecraft allow flexibility for the incorporation of such a spectrometer. Further study will include outlining a method for maximizing the resolution with a goal of obtaining 3000. This will also necessitate an effective area optimization study. As seen from the designs, the current grating arrays are small and easily manageable from all aspects including fabrication, assembly, integration and control during flight. This opens up the possibility of using a second grating array. A second set of gratings and CCDs would instantly open up many avenues for increasing resolution and throughput concurrently. However, more detailed work needs to be done to accurately account for the mass of these systems including the masses of the required CCD arrays, mounts, hardware, etc.

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