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ABSTRACT

The Off-plane Grating Rocket Experiment (OGRE) is a soft X-ray spectroscopy suborbital rocket payload scheduled for launch in Q3 2020 from Wallops Flight Facility. The payload will serve as a testbed for several key technologies which can help achieve the desired performance increases for the next generation of X-ray spectrographs and other space-based missions: monocrystalline silicon X-ray mirrors developed at NASA Goddard Space Flight Center, reflection gratings manufactured at The Pennsylvania State University, and electron-multiplying CCDs developed by the Open University and XCAM Ltd. With these three technologies, OGRE hopes to obtain the highest-resolution on-sky soft X-ray spectrum to date. We discuss the optical design of the OGRE payload.

Keywords: Optical design, X-ray spectroscopy, grating spectroscopy, diffraction gratings, X-ray optics

1. INTRODUCTION

The soft X-ray bandpass ($\sim 0.3 - 1.5$ keV) hosts a variety of astrophysically abundant absorption and emission lines. These transition lines provide a wealth of information about astrophysical plasmas and other highly-energetic astrophysical phenomena throughout the Universe. Advances in this regime would allow astronomers to begin to address many of the science goals laid out by the NASA Astrophysics Research Program. For example, a high-performance soft X-ray spectrograph would enable the study of high-energy stellar processes and their effects on protoplanetary disk formation and evolution, probe the most massive black holes residing at the centers of galaxies, and search for the missing baryons thought to reside in the warm-hot intergalactic medium.[1] The only instrument capable of high-performance spectroscopy in the soft X-ray bandpass is a grating spectrograph.

Current X-ray grating spectrographs onboard missions such as the *Chandra X-ray Observatory*[2] and *XMM-Newton*[3] have served the X-ray community well for the past several decades, enabling numerous advances in the field.[4,5] Emerging technologies will enable the next generation of X-ray spectrographs such *Lynx*[6] to realize order of magnitude performance increases over existing spectrograph missions, which will facilitate countless more advances. However, before inclusion on the next generation of X-ray spectrographs, these emerging technologies must first be proven on smaller mission architectures.

The Off-plane Grating Rocket Experiment (OGRE) is a soft X-ray grating spectrograph that will be flown on a suborbital rocket payload. Scheduled to launch in Q3 2020 from Wallops Flight Facility, OGRE will observe the double binary star system Capella, a line emission dominated astrophysical source in the soft X-ray bandpass, and aims to achieve the highest-resolution spectrum of this source to date (goal: $R(\lambda/\Delta\lambda) > 1500$). To achieve this

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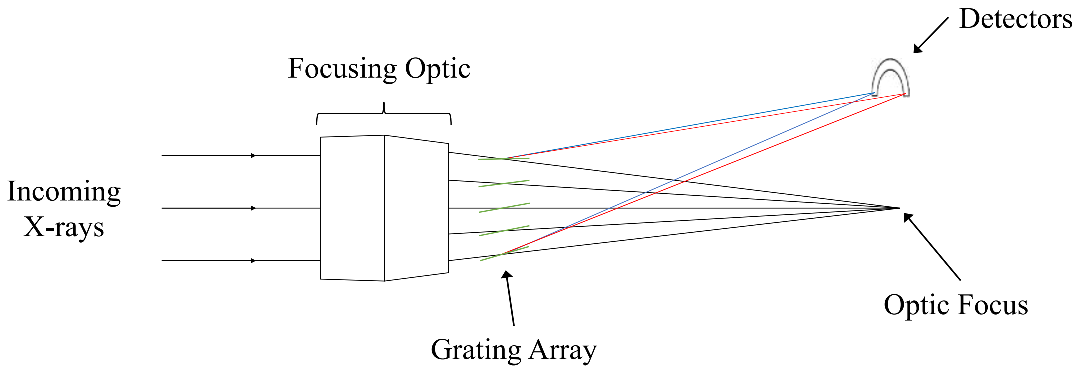

Figure 1. Schematic of a soft X-ray reflection grating spectrograph. Incoming X-rays are incident on a focusing optic, which forms a converging X-ray beam. This beam is intercepted by a reflection grating array, which diffracts the converging beam onto detectors located at the focal plane of the spectrograph.

high performance, OGRE will utilize three key technologies: X-ray reflection gratings, monocrystalline silicon X-ray focusing optics, and an array of electron-multiplying CCDs (EM-CCDs) at the focal plane. The suborbital rocket mission architecture provides these technologies an avenue to prove themselves in a space environment, but this mission architecture also places tight constraints on the design of the spectrograph. In this manuscript, we discuss the optical design of the OGRE payload.

2. THE OGRE SPECTROGRAPH

A soft X-ray grating spectrograph generally consists of three components: an X-ray focusing optic (typically Wolter-I type[7]), a grating array, and an array of detectors on the focal plane. A schematic of this spectrograph design can be seen in Fig. 1. X-ray photons from an astronomical source are incident on the two-part Wolter-I X-ray focusing optic, which forms a converging X-ray beam. This converging X-ray beam is then intercepted by an array of gratings (either transmission or reflection), which diffracts the light into its component spectrum on the spectrograph focal plane. An array of detectors is then placed at this focal plane to read out the observed spectrum. The OGRE payload will utilize advanced technologies in each of these areas to form its high-resolution spectrograph.

2.1 X-ray Optics

To achieve high resolving power, the line spread function at the detector must be as narrow as possible. The foundation of the spectral line shape in an X-ray spectrograph is the focus formed by the spectrograph's optic; therefore, X-ray spectrographs desire X-ray optics which produce narrow foci. One method commonly employed to narrow the width of the optic focus is to subaperture the optic, such that only a small ($30° - 60°$) azimuthal span of the X-ray optic is utilized by the grating arrays.[8] This results in a focus much wider in the plane of reflection than in the perpendicular direction. Additionally, high-resolution X-ray spectrographs employ X-ray optics which have high angular resolution, which results in a narrow optic focus at the focal plane. Traditionally, high angular resolution X-ray optics required thick optic substrates which could stand up to the intensive polishing processes needed to achieve the surface qualities desired.[9]

As a suborbital payload, OGRE has only a small window of time above the Earth's atmosphere to perform its scientific observation ($\sim$ 300 sec). Therefore, the spectrograph needs to be designed to collect as many photons from Capella as possible over its short observation time. Further, space-based missions, including the suborbital rocket mission architecture, have strict weight requirements due to the steep cost of lifting objects above the Earth's atmosphere. These requirements necessitate X-ray mirrors which are thin to allow a tight packing geometry for collecting as many photons as possible and lightweight to satisfy sounding rocket weight requirements. Traditionally, however, thin and lightweight X-ray mirror substrates have been unable to achieve the high angular resolution desired in high-resolution X-ray spectrographs.

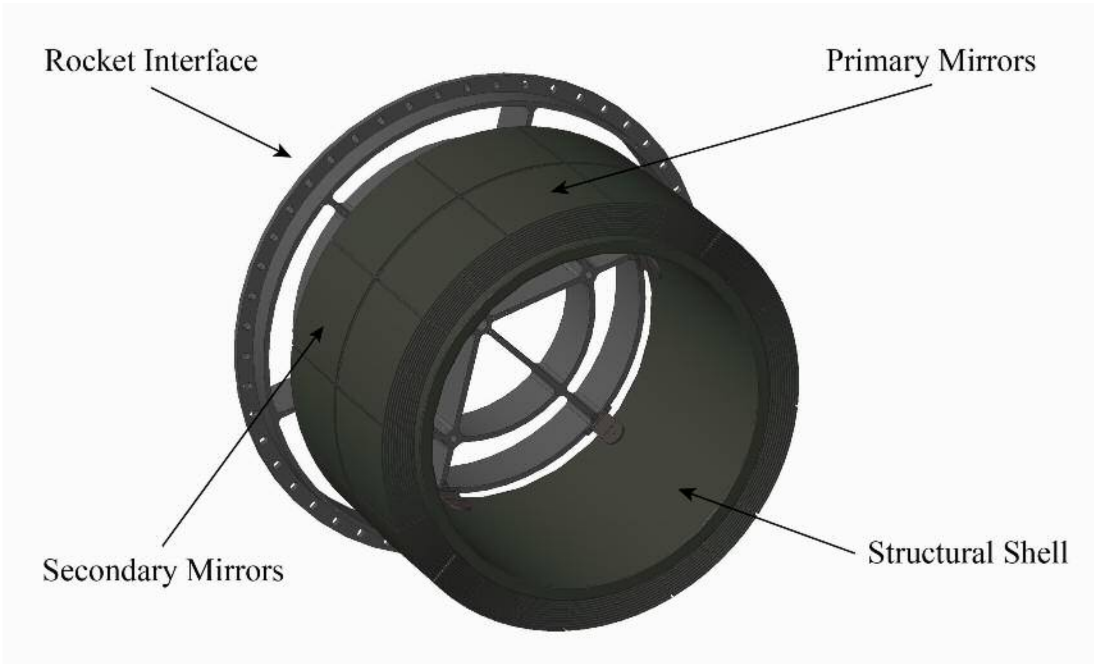

Figure 2. CAD model of the OGRE optics module. Seen are the 12 layers of monocrystalline silicon mirror segments both for the paraboloid (primary) and hyperboloid (secondary) surfaces which form the Wolter-I type optic. The mirror segments are mounted on a thick, structural shell, which interfaces with the internal optics bench on the payload.

Monocrystalline silicon X-ray optics developed at NASA Goddard Space Flight Center combine the high angular resolution and thin/lightweight attributes previously in conflict with each other to produce X-ray mirrors with high angular resolution in a thin, lightweight package.[10] Each mirror substrate still undergoes an intensive polishing process, but the substrate used (single-crystal silicon) and the specific polishing processes do not impart stresses into the mirror. This allows thin, lightweight mirrors to be produced with exceptional surface quality. The complete monocrystalline mirror manufacture process is described in detail in Riveros et al. 2017.[11] Once manufactured, the mirror segments are integrated onto a thick structural shell to form the X-ray mirror assembly. This process is known as the "meta-shell" approach.[12]

In a grating spectrograph, high spectral resolution ($R = x/\Delta x$) is obtained by both increasing the dispersion (x) of the photons from zero order and decreasing the width of the spectral line spread function at the focal plane (Δx). The monocrystalline silicon X-ray optics module utilized on OGRE hopes to achieve a point spread function (PSF) with ≤ 1 arcsec width FWHM in the dispersion direction ($60°$ azimuthal span) and a half-power diameter of $\sim 3-5$ arcsec. To increase the dispersion of a spectrograph, the grating array is typically placed as far away as technically feasible from the focal plane. Since the OGRE payload will be flown on a suborbital rocket, the allowable total payload length is severely constrained. The OGRE optics module will have a focal length of 3.5 m, which is the longest allowable focal length that can still maintain payload stability during launch. These optic attributes will provide a solid foundation to achieve a narrow line spread function at high dispersion, which is essential for the OGRE spectrograph to produce a high-resolution spectrum. The current CAD model of the OGRE optics module can be seen in Fig. 2. The module will utilize 12 shells of monocrystalline silicon mirror segments, ranging in diameter from 330 mm to 388 mm. In total, the optics module will contain ~ 260 mirror segments.

2.2 Grating Array

2.2.1 X-ray Reflection Gratings

The OGRE spectrograph will utilize reflection gratings as its dispersive element to separate the incident light into its component spectrum. Reflection gratings operated in the extreme off-plane mount have demonstrated

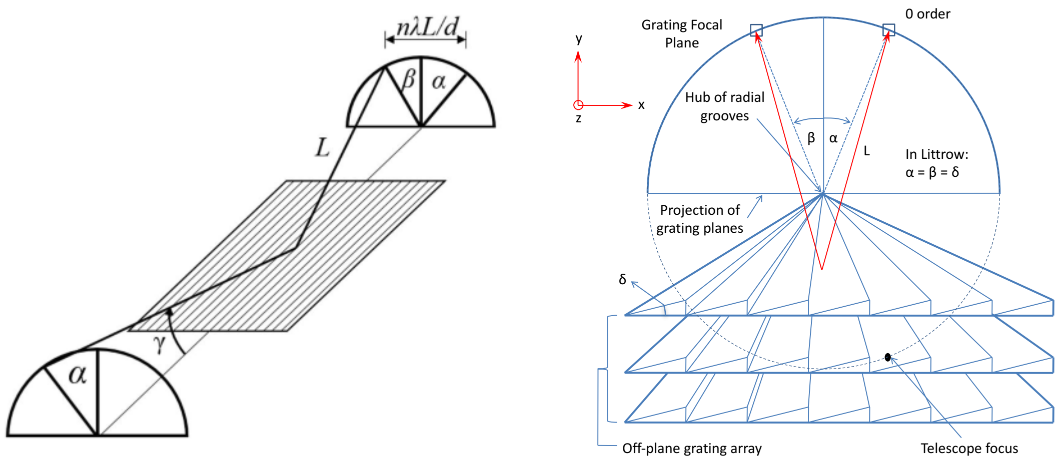

Figure 3. Reflection grating geometry in the extreme off-plane mount.[17] *(Left)* Light is incident on the grating quasi-parallel to the groove direction with a graze angle γ. Diffracted light is then directed toward the focal plane, following the generalized grating equation described in Eq. 1. *(Right)* An idealized array of three aligned gratings with a blazed groove profile in the Littrow mount ($\alpha = \beta = \gamma$).

high spectral resolution[13] and high diffraction efficiency[14] in the soft X-ray bandpass. Compared to the in-plane reflection geometry used on missions such as XMM-Newton, reflection gratings in the extreme off-plane mount are rotated approximately 90° about the grating normal such that the grating grooves are approximately parallel to the incident photons.[15] This grating geometry can be seen in Fig. 3 and is described by the generalized grating equation,

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

where γ is the polar angle of the incident X-rays of wavelength λ defined from the groove axis at the intersection point, d is the line spacing of the grooves, α is the azimuthal angle along a cone with half-angle γ, β is the azimuthal angle of the diffracted light, and n is the diffracted order.[16]

Reflection gratings in the X-ray bandpass operate at grazing incidence ($\gamma \leq 2°$), which reduces the collecting area of the grating surface tremendously. Typical reflection gratings are $\sim 100 \times 100$ mm^2, which reduces to $\sim 2.6 \times 100$ mm^2 at an incidence angle of 1.5 degrees. To reclaim the collecting area lost by operating at grazing incidence, reflection grating spectrographs utilize co-aligned arrays of gratings such that their individual diffraction arcs overlap at the focal plane.

Reflection gratings can be manufactured with blazed, or triangular, groove profiles. This serves to preferentially disperse the diffracted light in the direction normal to the groove facet, as seen in the right-hand panel of Fig. 3. Reflection gratings with a blazed groove profile allow spectrographs to operate at high dispersions to achieve high spectral resolution, while maintaining high throughput. Reflection gratings can also be manufactured with a radial groove pattern such that all grooves converge at the center of the diffraction arc; this serves to reduce aberrations on the focal plane when operated in the extreme off-plane mount and therefore increase the resolution of the spectrograph. The current state-of-the-art reflection gratings are manufactured at The Pennsylvania State University in its Materials Research Institute, with a detailed discussion found in McCoy et al. 2016.[18]

2.2.2 Grating Design

As mentioned previously, X-ray spectrographs generally subaperture their X-ray optic such that only a small ($30° - 60°$) azimuthal span of the optic is populated with grating arrays. This serves to decrease the width of the

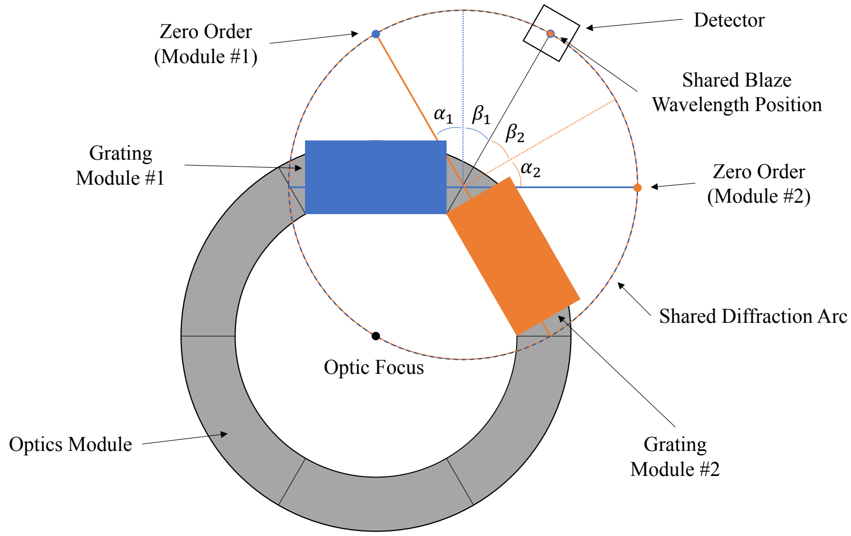

Figure 4. Schematic of the grating module diffraction geometry for the OGRE spectrograph. Shown here are two of the six grating modules which populate the full 360° azimuthal span of the OGRE optics module. Each grating module fills a 60° azimuthal segment of the optic. Pairs of grating modules are manufactured to operate in opposite Littrow configurations so as to preferentially diffract their incident light to the same location on the spectrograph focal plane.

X-ray focus in the dispersion direction, which in turn decreases the width of the spectral lines at the spectrograph focal plane and increases spectral resolution. For OGRE, however, the entire 360° azimuthal span of its optics module needs to be covered with grating arrays to maximize the flux seen during its short observation time. Therefore, an alternative solution to the traditional telescope subaperturing technique was needed for OGRE.

The OGRE optics module will be split into six 60° azimuthal sections with a grating module placed behind each of these sections. Thus, the OGRE spectrograph will have six separate diffraction arcs. This solution maintains the subapertured optic beam needed to obtain high resolution, while also maximizing flux by utilizing the full azimuthal span of the optic. Neighboring 60° azimuthal sections of the optic are populated with grating arrays with opposite yaws, which allows these neighboring sections to preferentially diffract their light to the same location on the focal plane. A schematic of this concept can be seen in Fig. 4. This solution reduces the required number of spectral detectors from six to three. Further, each grating array is either identical to or a mirrored version of every other grating array in the OGRE grating module, simplifying the grating fabrication and alignment processes.

To maximize diffraction efficiency, OGRE gratings will operate in the Littrow mount ($\alpha = \beta = \delta$).[19] For each 60° azimuthal section of optic, $\alpha = \beta = 30°$. The angles in Fig. 4 then become $\alpha_1 = \beta_1 = \alpha_2 = \beta_2 = 30°$. To satisfy the Littrow mounting condition, the grating grooves then must be blazed to $\delta = 30°$.

While the Littrow mount maximizes diffraction efficiency for a blazed grating, the diffraction efficiency must be maximized around the wavelength of interest for OGRE ($8 - 42$ Å). The Littrow mount maximizes diffraction efficiency at the blaze wavelength:

$$\lambda_b = \frac{2d \sin\gamma \sin\delta}{n}. \tag{2}$$

For the above diffraction geometry and wavelength of interest, the groove period for the OGRE gratings must be $d \approx 160$ nm. The grating parameters presented here are in agreement with currently produced reflection gratings at The Pennsylvania State University.

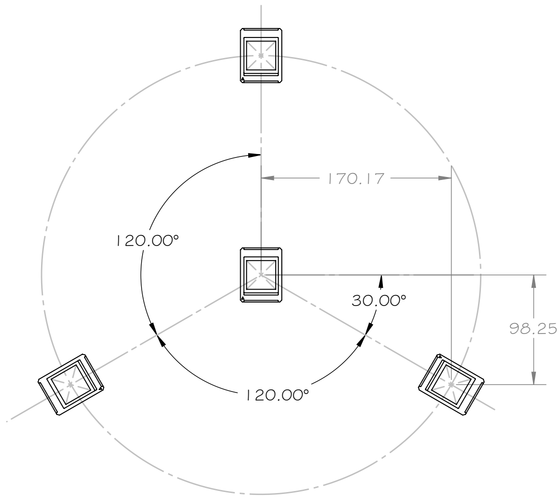

Figure 5. Layout of detectors on the focal plane. The spectral detectors are centered at the blaze wavelength of the instrument and are clocked 120° with respect to each other as each detector shares spectra from two 60° azimuthal optic segments. The telescope focus detector lies along the optical axis of the optics module.

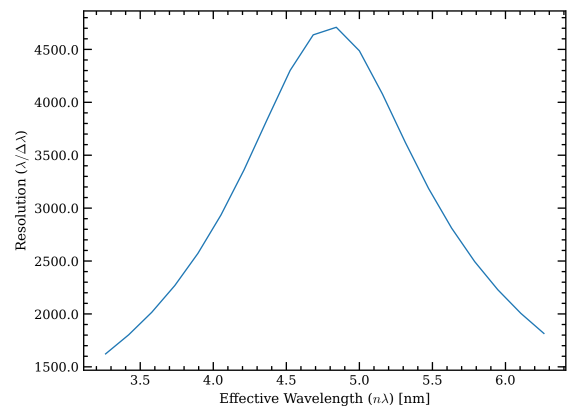

Figure 6. Theoretical resolution response of the OGRE spectrograph around the effective blaze wavelength ($n\lambda_b = 4.76$ nm). The resolution of the spectrograph peaks around the blaze wavelength, where spectral detectors were placed to maximize observed resolution, and falls off rapidly outside the wavelength of interest due to path length differences.

Each 60° azimuthal section of optic contains two columns of ∼75 x 100 mm^2 gratings stacked to cover the entire radial span of the optics module. These dimensions were chosen to minimize the number of gratings to align, while maximizing the yield from a standard 6-inch diameter wafer. Grating positions were determined via numerical raytrace optimization to maximize spectral resolution at the blaze wavelength. The final grating design requires ∼ 200 gratings to fully sample the converging beam from the optics module.

2.3 Focal Plane

The final component of a reflection grating spectrograph is a detector array at the spectrograph focal plane. This focal plane must be placed in the correct position so as to minimize the path length differences of photons diffracting off the individual gratings. At this position, the highest spectral resolution is achieved. This focal plane is generally angled relative to the telescope focal plane, as the grating coordinate system is rotated relative to the telescope coordinate system.

OGRE will utilize four detectors: three will each image two of the six diffraction arcs (as demonstrated in Fig. 4) and one will observe the telescope focus formed by the remaining photons not intercepted by the grating arrays. The telescope focus detector is placed at the telescope focal plane, 3500 mm from the intersection plane of the optics module. Each of the three spectral detectors will monitor two diffraction arcs simultaneously and will be centered at the shared blaze wavelength of these two diffraction arcs. The positioning of all four detectors on the focal plane can be seen in Fig. 5.

Since each spectral detector will monitor two diffraction arcs, it must be placed to minimize the path length differences of the two diffraction arcs simultaneously. This location was numerically determined via raytrace simulations and bisects the spectrograph focal planes of the two grating modules it observes. This spectrograph focal plane configuration reduces the obtainable resolution of the spectrograph far away from the blaze wavelength due to path length differences (one grating module will be intrafocal and the other extrafocal), but will maintain high resolution around the blaze wavelength and the wavelength of interest. The theoretical resolution response for OGRE around its blaze wavelength ($n\lambda_b \approx 4.66$ nm) can be seen in Fig. 6. This idealized resolution response assumes an optic performance of ≤ 1 arcsec FWHM in the dispersion direction and perfect alignment of all elements in the spectrograph. In reality though, the maximum resolution seen in Fig. 6 will decrease due to a variety of factors, including in-flight pointing knowledge, grating misalignments, grating period errors, etc. However, this theoretical resolution response serves as an excellent starting point for achieving the OGRE mission goal of $R > 1500$.

3. SUMMARY

The Off-plane Grating Rocket Experiment aims to achieve the highest-resolution astronomical soft X-ray spectrum to date when it launches in Q3 2020. The suborbital rocket mission architecture places severe constraints on the design of such a spectrograph, yet a high-resolution spectrograph which can theoretically achieve the resolution goal of $R(\lambda/\Delta\lambda) > 1500$ over the wavelength of interest has been devised (Fig. 6). The spectrograph will utilize a high angular resolution optics module consisting of 12 shells of monocystalline silicon optics feeding an array of reflection gratings. The spectrograph is unique in that the grating arrays sample the entire 360° azimuthal extent of the optic and form six distinct diffraction arcs. Three spectral detectors each sample two of the six diffraction arcs and a fourth detector samples the remaining photons not intercepted by the grating modules.

4. FUTURE WORK

This manuscript laid out a general overview of the optical design of the OGRE spectrograph. Much of the remaining work left to be completed concerning the spectrograph's optical design relates to grating alignment tolerances and a comprehensive line spread function error budget. Rough grating alignment tolerances can be calculated by following the formalism laid out Allured & McEntaffer 2013,[20] however this analysis leads to overly optimistic alignment tolerances as it does not consider multiple degrees of freedom simultaneously. In reality, all six degrees of freedom must simultaneously be monitored via raytrace simulations to derive robust alignment tolerances for the OGRE grating modules. These alignment tolerances will then be incorporated into a comprehensive line spread function error budget, which itemizes each individual contribution to the final dispersed line spread function on the OGRE focal plane. This includes grating alignment tolerances, grating flatness, optic performance and alignment, and other misalignments in the spectrograph. With accurate errors in the error budget, it can then be used to predict the expected performance of the OGRE spectrograph and update the resolution response of the spectrograph (Fig. 6). The error budget will be devised such that the spectrograph achieves its goal of $R > 1500$.

The design of the OGRE optics module has already been finalized and work has begun to produce prototype mirror segments for the innermost Wolter-I shell. Once this prototype mirror pair has been completed, it will be tested for performance at The Pennsylvania State University to ensure it meets the requirements of the OGRE payload. At that point, production of the OGRE optics module will begin. The OGRE focal plane design is also close to being finalized, with production set to commence once this design has been finalized. Finally, prototype off-plane gratings have been manufactured at The Pennsylvania State University and its Materials Research Institute. These gratings are currently being tested at Penn State to verify their performance, at which point flight gratings will be produced and aligned into grating modules.

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