Development of off-plane gratings for WHIMex and IXO

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ABSTRACT

Future X-ray astronomical missions will need to address a number of important goals such as studying the dynamics of clusters of galaxies, determining how elements are created in the explosions of massive stars, and revealing most of the "normal" matter in the universe which is currently thought to be hidden in hot filaments of gas stretching between galaxies. In order to achieve these goals, spectrometers capable of high resolution and high throughput are necessary for the lowest X-ray energies, 0.3-1.0 keV. We present recent progress in the development of off-plane reflection grating technology for use on upcoming missions. Off-plane grating spectrometers consist of an array of gratings capable of reaching resolutions above 3000 ($\lambda/\Delta\lambda$). Concept designs have been made for the International X-ray Observatory X-ray Grating Spectrometer. More recently however, we have designed an Optics Module Assembly for WHIMex, an Explorer mission concept that incorporates a Wolter telescope, steering flats, and an array of gratings. This paper will discuss these designs and the application of off-plane arrays for the future.

Keywords: X-ray Spectroscopy, off-plane gratings, International X-ray Observatory, WHIMex

1. INTRODUCTION

The International X-ray Observatory (IXO) baseline configuration includes an X-ray Grating Spectrometer (XGS) instrument. The purpose of the IXO XGS is to provide high spectral resolution, $\lambda/\Delta\lambda > 3000$, and high effective area, >1000 cm^2, at low energies 0.3-1.0 keV. This represents more than an order of magnitude increase in effective area together with an increase of approximately an order of magnitude in resolving power over previous observatories. This huge increase in performance will open up new discovery space, and in particular will address key scientific questions such as;

- Measurements of the WHIM
- Velocity distributions e.g. in AGN outflows
- High resolution line emission from stellar atmospheres and plasmas

However, the recent Astro2010 Astronomy and Astrophysics Decadal Survey deemed IXO unready for flight and in need of significant technology demonstration in the next decade. With the aging of current observatories such as the *Chandra* X-ray Observatory and *XMM-Newton*, the field of X-ray astronomy is in jeopardy of realizing an absence of an appropriate scientific workhorse for the field. Given the delay in IXO, a suitable plan for the short-term is to develop smaller missions that can fit into a NASA Explorer program yet be capable of accomplishing some of the key science

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goals of IXO. Here we present the progress of one such mission, the Warm Hot Intergalactic Medium Explorer (WHIMex). The design leverages heavily from developments made during the IXO project. The spectrometer utilizes the same elements yet in a dedicated grating spectroscopy package.

2. IXO DEVELOPMENTS

2.1 Technology Description

Here we describe a reflection grating concept known as the Off-Plane X-ray Grating Spectrometer (OP-XGS)[1]. The design utilizes an array of gratings in the off-plane configuration and a CCD camera for the readout. The technologies are very similar to those utilized for *XMM-Newton* and also have heritage in suborbital rocket missions.

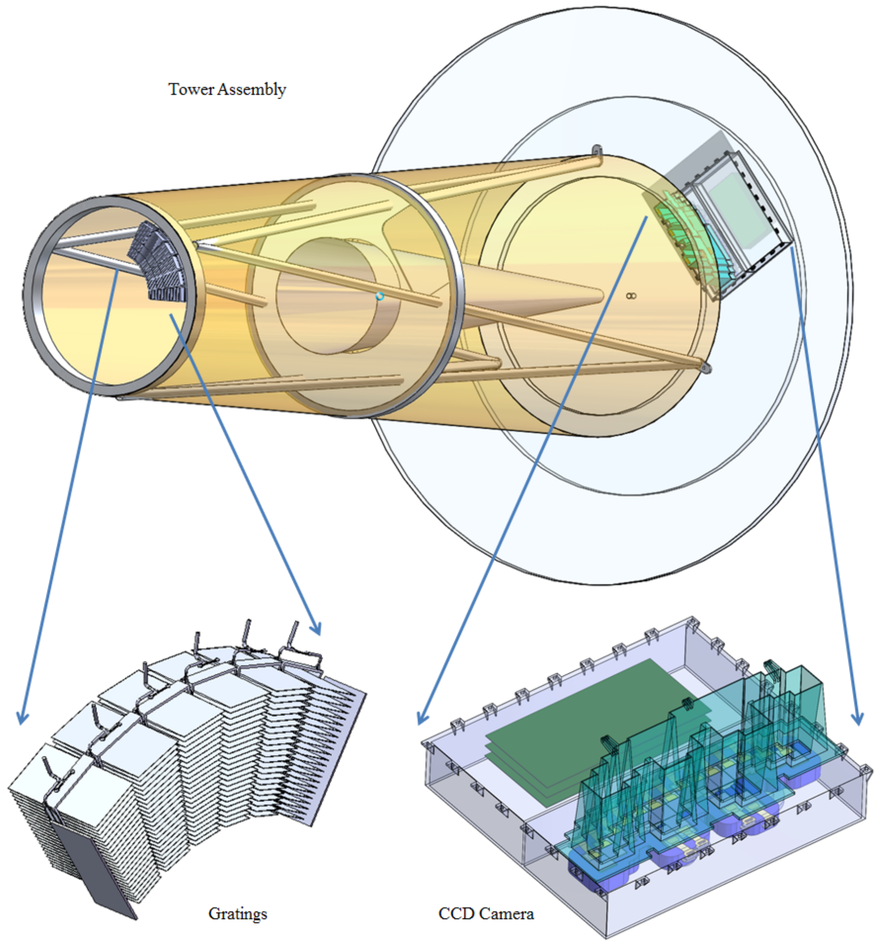


Figure 1: Schematic of the OP-XGS concept design. Six grating modules are placed on a tower assembly extended from the instrument platform which also houses the readout CCD camera.

The instrument consists of an array of reflection gratings in the off-plane mount that intercepts a small portion of the main telescope beam and diffracts the light onto an array of dedicated CCDs. The Off-Plane configuration is capable of meeting the instrument performance requirements at any position along the IXO optical axis from just aft of the optics (focal length = ~19 m) to just a few meters away from the focal plane. This parameter space has been studied in depth to achieve an optimal configuration for the present IXO spacecraft design in which the grating array is placed 5.16 m from the focal plane via the use of a lightweight structural tower.

An example layout is shown in Figure 1. The OP-XGS comprises a grating array mounted upon a rigid lightweight tower which itself is mounted on the instrument platform. The tower can also serve as the support for the baffle for the on-axis instruments, providing some saving in system resources. The length of the tower can be tuned to meet the observatory design. The grating array diffracts a portion of the beam (approximately 10%) into several arcs, or spectra, into a fixed

CCD camera. The camera is mounted on the instrument platform and consists of an array of CCDs with associated electronics, thermal control and radiation, stray light and contamination shielding.

The Grating System consists of a Grating Array made from 6 separate, yet identical, modules as visible on the bottom left detail of Figure 1. These grating modules are mounted to the top of the Grating Tower along with an independent thermal control system. Each of the 6 modules contains 23 gratings that differ only by their width and are co-aligned to form a single spectrum per module. The grooves on these gratings lie nearly parallel to the direction of the incoming X-rays (the off-plane mount) and exhibit a radial, blazed, high density profile that allows them to obtain high throughput and high resolution. A key element in the instrument design is the detailed layout and groove specification of the gratings themselves. The fabrication of the gratings is achieved through an industrial process which has been well established and therefore represents a low risk and manageable technology development/procurement.

The CCD camera draws upon the significant heritage of the X-ray cameras which are successfully employed on XMM RGS and EPIC, and Chandra ACIS. Due to the spectra having very high resolution, it is not possible to superimpose the outputs of the 6 grating modules onto a single spectrum, and instead we project 6 separate spectra onto the CCD camera. The overlapping spectra provide a high degree of redundancy in the design, where individual CCDs or their drive electronics can be lost without significantly impacting the science data return.

A number of advantages arise from the Off-Plane geometry in this configuration:

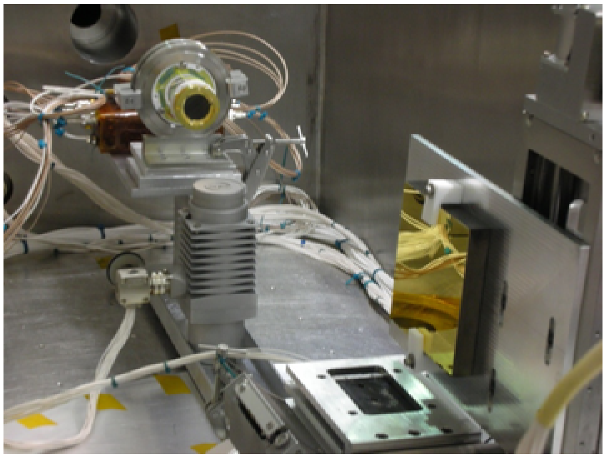
- Meets the science requirements with flexibility to accommodate changes in observatory performance as the spacecraft design evolves
- Meets the A_{eff} requirement of >1000 cm^2 in the 300-1000 eV band and exceeds the requirement at other energies – average A_{eff} across bandpass >1500 cm^2
- Has extended performance out to 1500 eV due to the efficiency of the gratings and CCDs at the higher energies
- Meets spectral resolution requirement with >20% margin and resolutions upward of 7000
- No scatter into focal plane instruments
- Compact camera design reduces mass requirements
- Large depth of focus enables focusing by observatory without additional focusing mechanism
- The tower structure provides a convenient and mass-efficient means for integration of other IXO components such as common baffle and particle deflectors for focal plane instruments
- The system is multiply redundant in the 6 individual spectra projected onto the camera, the electronics concept, CCD array, and thermal control systems

A strength of the design is that it is underpinned by relatively mature technology for the key components of gratings and CCDs. This design ensures a high TRL for the OP-XGS instrument, which in-turn will help ensure delivery on-time and to-budget. The grating consortium is academically-led from institutes with a strong track record in such instrumentation (Universities of Iowa and Colorado in the US, and Open and Leicester Universities plus MSSL in the UK) and is backed by industrial collaborators with strong space heritage (Northrop Grumman and e2v technologies).

2.2 Progress, Status and Plan

Off-plane gratings have flown on a number of suborbital missions and provide heritage for the design presented here[2,3]. Furthermore, the grating substrates, grating modules, alignment technique, and CCD camera are very similar to those used for *XMM*. To date, the technology development specific to IXO has concentrated on meeting the efficiency and resolution requirements for the gratings. A combination of analytical predictions, extensive raytracing, and laboratory demonstrations show that the design is capable of obtaining the performance requirements for IXO.

Theoretical calculations of grating efficiency performed independently by the grating manufacturer, Horiba Jobin-Yvon, and our team give expected efficiencies at the 50% level, sum of orders. Using a radial, blazed, high density prototype grating we have empirically obtained grating efficiencies >40%, thus approaching theoretical. The current design provides >1000 cm^2 of effective area from 0.3-1.0 keV assuming a 40% grating efficiency. An example of the efficiency testing facilities is shown in Figure 2.



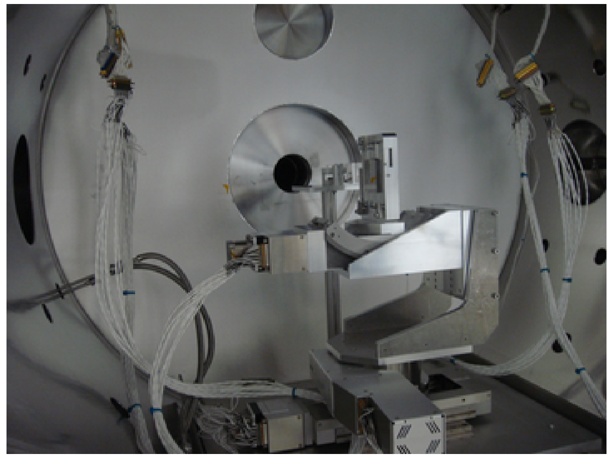


Figure 2: Test grating in the University of Colorado X-ray Test Facility (left) and in the University of Iowa Facility (right).

Raytrace analysis of the design gives a theoretical resolution of 9000 ($\lambda/\Delta\lambda$) at 1 keV in 3rd order. Using a radial, blazed grating we have empirically achieved a resolution of >200 at 1 keV with a 3' telescope. Extrapolation to a 5" telescope gives a spectral resolution of 7200, well above the requirement of 3000 over the bandpass. An example of an off-plane grating in a resolution test setup, complete with GSFC slumped glass Wolter optics, is shown in Figure 3. This configuration, along with a soft X-ray CCD camera (not shown), was recently used in testing at the MSFC Stray Light Facility.

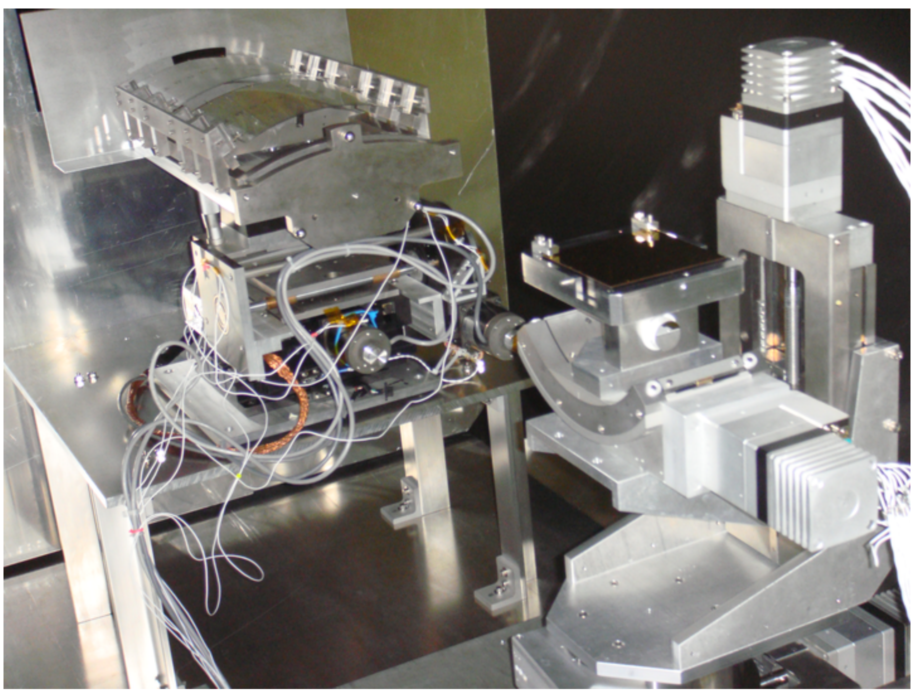


Figure 3: The MSFC Stray Light Facility large vacuum chamber with test optics. In the upper left of the image a single parabola and hyperbola are held in a kinematic mount. The test grating apparatus is located on right side of the image with 4-axis motion control.

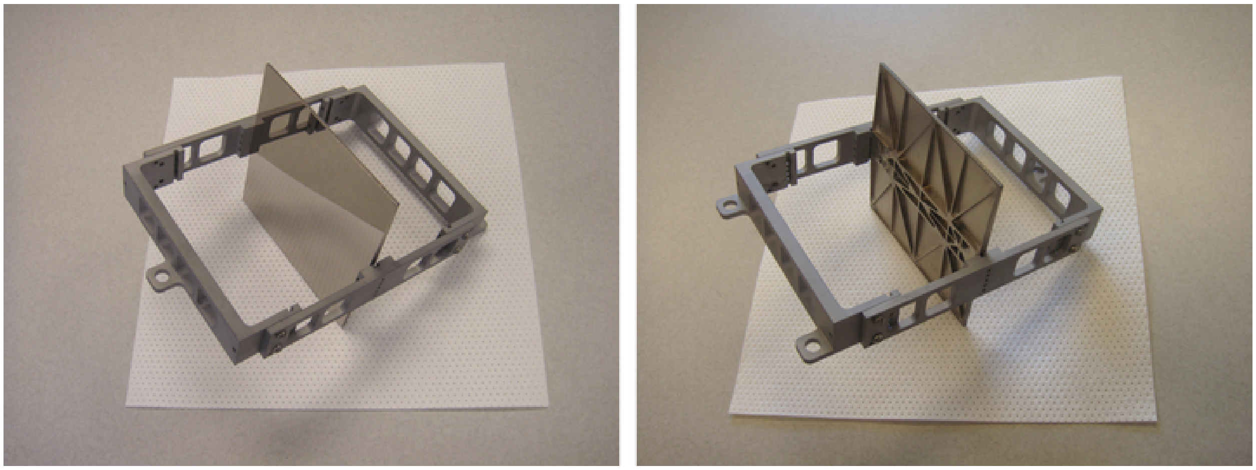


Figure 4: A high fidelity Be grating substrate assembled with a Be grating module mount. The image on the right shows the polished reflective surface while the image on the left is the lightweighted back side.

All tests have been performed in a relevant environment in terms of temperature and pressure with X-rays, but vibration tests have not yet been performed.

Development has continued in structural modeling and fabrication. Specifically, high fidelity grating substrates and grating module mounts have been fabricated. Figure 4 shows an assembly of a single grating substrate in a module mount. All parts shown have are precision machined Be providing a lightweight, stiff assembly with no CTE mismatch. The grating substrates have a polished Ni surface with a $\lambda/4$ figure and <1 nm roughness. The substrate profile is trapezoidal and lightweighted on the back as seen on the right side of the image. These substrates are very similar in form and function to those in the XMM-RGS. The proposed OPXGS concept design incorporates identical substrates in terms of material, size, mass, and surface quality. The module design provides 6 degrees of freedom for manipulation of the gratings. This prototype design allows for 3 gratings to be aligned. Alignment protocols, metrology, and testing are the next steps in module technology development.

2.3 Development Milestones

The two key technology development efforts for the OP-XGS will be in grating fabrication and optical filtering of the CCDs.

The grating fabrication development begins with the fabrication and testing of a flight prototype grating master. The grating will have a radial groove profile with high density blazed gratings. X-ray efficiency and spectral resolution verification tests on this master and replicas of the master are necessary to demonstrate TRL 4. Replicas will be imprinted onto medium fidelity grating substrates. Efficiency testing will be performed at the University of Iowa with resolution testing in the Stray Light Facility at Marshall Space Flight Center.

The demonstration of TRL 5 requires environmental and X-ray testing of a replica in a medium fidelity grating mount. Verification of performance and alignment pre and post environmental testing will be key steps in achieving TRL 5. Following TRL 5 development, the demonstration of an aligned high fidelity grating module will be required for TRL 6. The component fidelity will be increased for the groove profile, grating substrates, grating module mount, and alignment technique. Several replicas (3-5) will be assembled into a module with co-aligned X-ray spectra. Efficiency testing of this assembly as well as pre and post environmental resolution and alignment testing will be key steps. In addition, we will fabricate a prototype tower structure for use in these alignment tests.

The CCD filter technology development plan includes the following steps. The first step is procurement of a set of filters/CCDs from e2v technologies. The detail of the procured filters is to be determined but may include CCDs in which half the active area has a filter applied and half is without. A subset of these CCDs will be set aside for long term storage/stability tests. We define successful testing at room temperature as achieving TRL 4, and cryogenic testing under vacuum as achieving TRL5. In practice these test results may be conducted in a single step (i.e. under vacuum at -80°C).

The test CCDs/filters will be tested at a CCD level for broadband attenuation to optical light, thus performing an A/B comparison for the coated and un-coated halves. The filters will be tested as a function of wavelength at facilities such as NPL, UK. The modeled X-ray transmission at soft X-rays will be confirmed using testing at a facility such as BESSY/PTB. Successful experimental demonstration of key performance parameters will demonstrate TRL 4 – with testing conducted at (or close to) room temperature. The CCDs will then be subjected to environmental testing including representative thermal (i.e. -80°C) tests under vacuum for low noise performance, thus providing a repeat of the optical/X-ray testing, mechanical testing, as well as results of the long term storage exercise. The key item for long term storage would be to check for a change in the thickness of the aluminum oxide on the filter, which would alter the optical and X-ray transmission properties. Successful evaluation will lead to TRL 5.

3. WHIMex OVERVIEW

3.1 Technology

An overview of the WHIMex spacecraft design is shown in Figure 5. The WHIMex spacecraft consists simply of a soft X-ray spectrograph. Two Astro-Booms are used to extend an Optics Module away from the focal plane CCD camera which is located in the Instrument Module (shown with attached solar panels). To obtain the science goals of characterizing absorption features due to the Cosmic Web, mapping AGN outflows, and measuring properties of extreme environments in our galaxy, WHIMex has the following performance requirements:

- Soft X-ray energy waveband, 0.2-0.8 keV
- High spectral resolution, >4000 ($\lambda/\Delta\lambda$)
- High quality optics, 15” telescope subapertured to 1.5”
- High sensitivity, effective area >250 cm^2

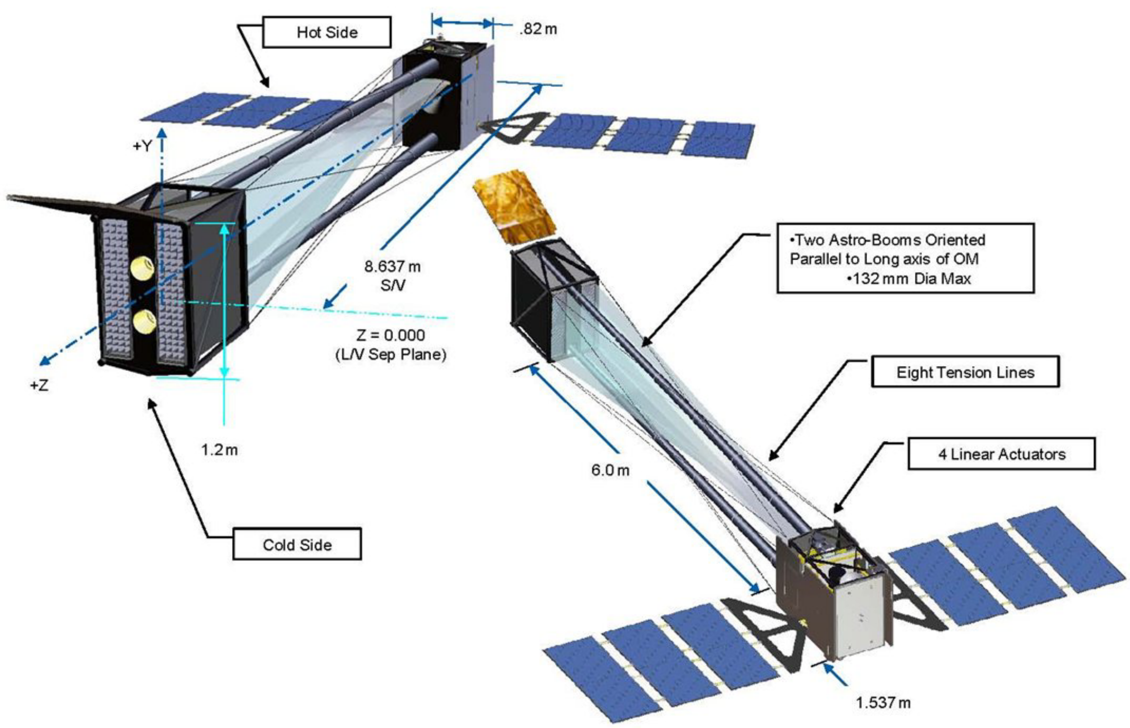


Figure 5: Spacecraft concept for WHIMex. On the left side the Optics Module is pointed out of the page.

The Optics Module forms the basis of the WHIMex concept. A schematic detailing the components in shown in Figure 6. The 4 reflection configuration represents a novel optical design. This design was driven by the desire to use identical parabola and hyperbola (P/H) pairs in the Wolter Type 1 telescope. This circumvents the budget and time issues involved with procuring many high precision forming mandrels used during the glass slumping process. With identical radii of curvature for all parabolas and hyperbolas only one prescription for the expensive mandrels is necessary as opposed to a separate mandrel for every annulus of mirrors in a typical X-ray telescope such as *Chandra* or *XMM*. Instead of nested annuli of optics, WHIMex uses parallel stacks of optics. Each optical element spans a limited range of azimuths (<60°) thus allowing for this configuration.

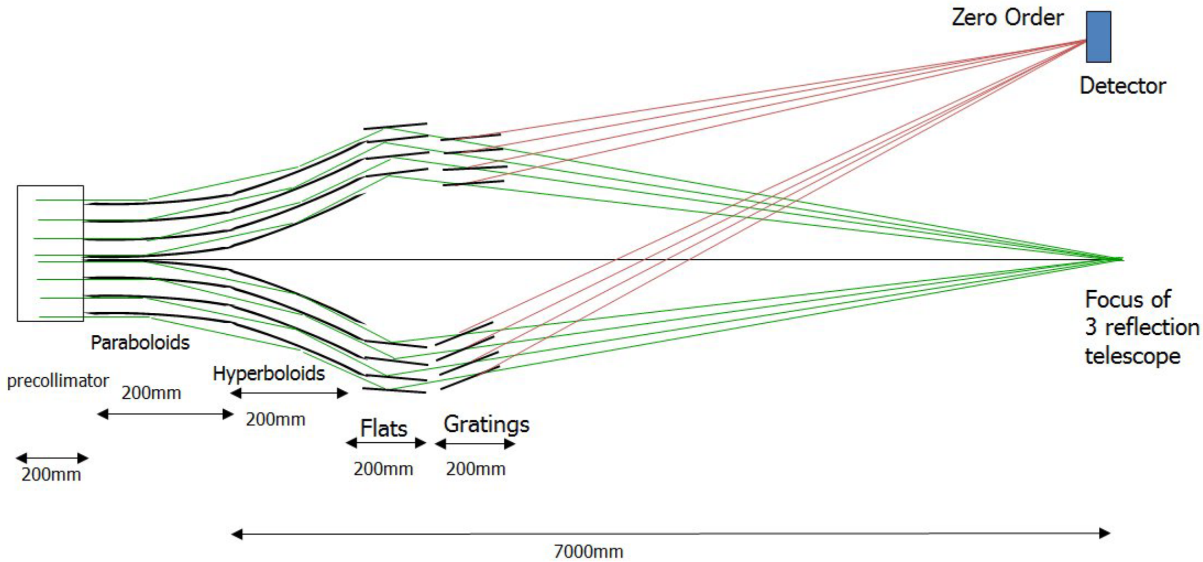
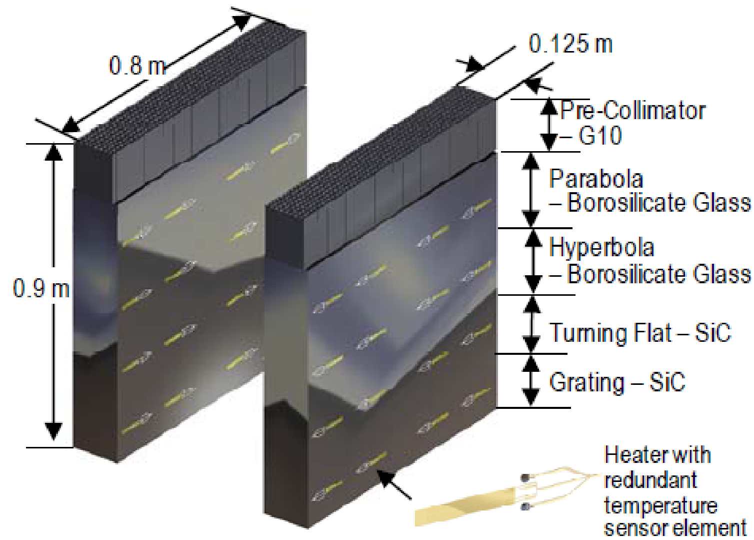


Figure 6: Schematic of the optics module. The module consists of a parallel stack of P/H pairs, followed by an array of steering flats and ultimately an array of gratings. The gratings disperse the spectrum orthogonal to the plane of the page onto an array of CCD chips.

The parallel stacking of the P/H pairs creates a collimated beam exiting the telescope. A set of "tuning" or "steering" flats is then used to overlap the foci from each pair creating a common focus. The additional reflection does little to limit the throughput of the design given that the graze angle on the P/H optics is 0.5° and the average graze angle on the flats is similar. A Ni coating and shallow graze angle ensure high reflectivity and throughput. Finally, an array of reflection gratings is fanned behind the optics to create the spectrum on an array of CCD chips. The gratings are fanned to maintain a constant graze angle on the gratings and therefore a constant γ (and α to some extent) in the grating equation,

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

This aids in maintaining a constant β for a given wavelength thus limiting any aberrations due to the grating groove profile. To remove further aberrations the groove profile for the gratings must match the convergence of the focused beam. This ensures a constant α over the width of the grating and hence constant dispersion per wavelength. This is the same concept being utilized for the IXO OP-XGS. In fact, aside from the steering flats, the optical elements for WHIMex are identical to those proposed for the OP-XGS. A CAD model of the Optics Module is shown in Figure 7. The aspect ratio demonstrates the high density packing geometry of the design (long axis) in addition to the limited azimuth of the optics (short axis, 125 mm). The limited azimuth not only allows for efficient packing, but it also exploits the concept of subaperturing the telescope beam. A significant fraction of a telescope HPD is due to scattering off the optics which is preferentially in the plane of the incoming light. Therefore, sub-sampling the azimuthal range of optics also sub-samples this scatter function thus resulting in a tighter telescope HPD in the off-plane direction. Dispersing along this direction using the off-plane mount thus maximizes the spectral resolution available in such a design.



Component	Number
Precollimator	2
Parabola/Hyperbola pairs (X-ray mirrors, 0.4 mm thick)	592 pairs, 1184 elements
Turning flats (1 mm thick)	592
Gratings (1 mm thick)	592
Thermal Control Subsystem	64 heaters, 128 sensors
Structure	2

Figure 7: A CAD model of the Optics Module. The assembly consists of 2 channels of 4 reflecting optics – a parabola, hyperbola, flat, and grating. The module will operate at 20° C which is maintained by the Thermal Control Subsystem.

Figure 8: Left - Precision optic formed through glass slumping during the IXO program. Right – test results from a permanently bonded P/H pair mounted in a housing simulator. The telescope HPD is 9.7” at 4.5 keV with a 1.4” subapertured FWHM.

As shown in Figure 7, the temperature of the Optics Module is controlled via a Thermal Control Subsystem. The operating temperature is nominally 20° C. The total production volume is ~1200 telescope elements, ~600 optical flats, and ~600 grating replicas. Given the heritage of the IXO project and the techniques developed during the last decade, this is well within the budget and time scope of an Explorer mission. Figure 8 shows one of the many optical elements formed through the glass slumping process studied during IXO. Note the relatively small range of azimuth covered per element. Also shown in this figure are empirical results from the testing of these optics. A P/H pair was permanently bonded in a housing simulator and produced a focus with 9.7" HPD as shown at the upper right. This is well within our goal of a 15" telescope leaving much room for element to element alignment. Furthermore, note the characteristic bowtie image. This results from the subaperture effect from the limited azimuthal range. The FWHM of the focus in the off-plane direction is on 1.4" thus allowing for high spectral resolution once this beam is dispersed. The gratings are very similar to those proposed for the IXO OP-XGS and will be reflection gratings in the off-plane mount. The groove profile is high density, 5500 gr/mm and blazed at 24°. The grooves have a radial profile (density increases toward the focal plane) to match the convergence of the telescope beam.

3.2 Expected Performance

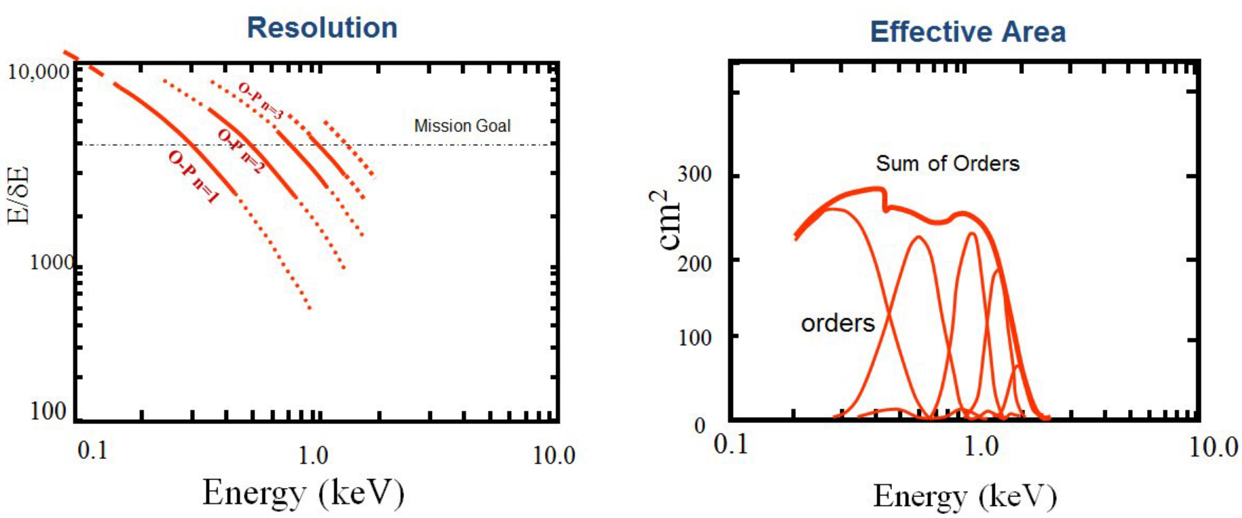


Figure 9: Expected performance of WHIMex based on detailed raytrace analysis.

The expected performance of WHIMex was determined based on detailed raytrace analysis of the entire Optics Module. The performance parameters are shown in Figure 9. The resolution goal of 4000 is met in first order at long wavelengths. Higher orders are necessary at higher energies due to the constant dispersion with wavelength. This is complemented by the fact that the blaze on the gratings places most of the light at these higher energies into higher orders. An example of the raytrace is given in Figure 10. The zero order image on the upper left displays the characteristic bowtie shape. The gratings are blazed to optimize 70 Å in first order. Each group of lines in the figure differ by 0.035 Å yet are separated by >2 resolution elements as seen from the plot on the upper right. This produces resolutions >4000 ($\lambda/\Delta\lambda$) around the blaze wavelength and longward. The spectrum at the focal plane was also raytraced. This is shown in Figure 11. Each channel of the Optics Module has a unique zero order. The gratings are blazed in opposite directions as well giving opposite dispersion directions. This results in a compact geometry for the CCD array. Furthermore, this gives spectral redundancy to the CCD camera. If a chip should fail, then only 50% of the data in that waveband would be lost as opposed to 100%. This CCD camera also leverages heavily from developments made for IXO. The CCDs are inherently at a higher TRL relative to the rest of the payload, but the technology for deposition of thin optical filters still needs to be developed.

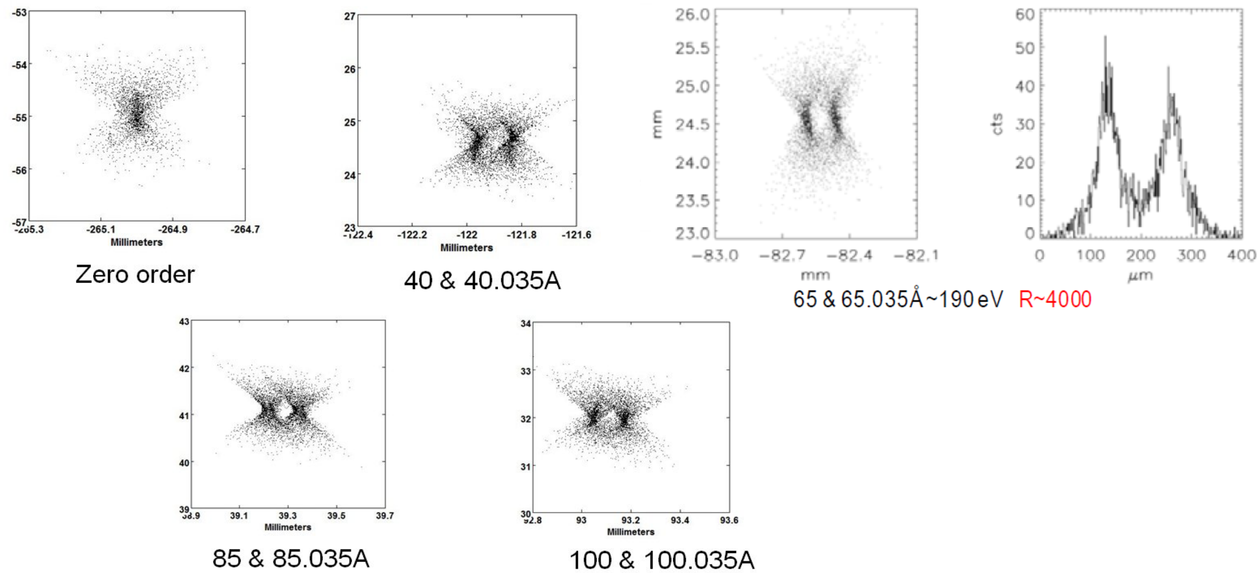


Figure 10: Spot raytraces at various wavelengths. Each pair of spots is separated by 0.035 Å. Each set of spots is clearly separated by > 2 resolution elements leading to resolutions of >4000 around the blaze wavelength and longward.

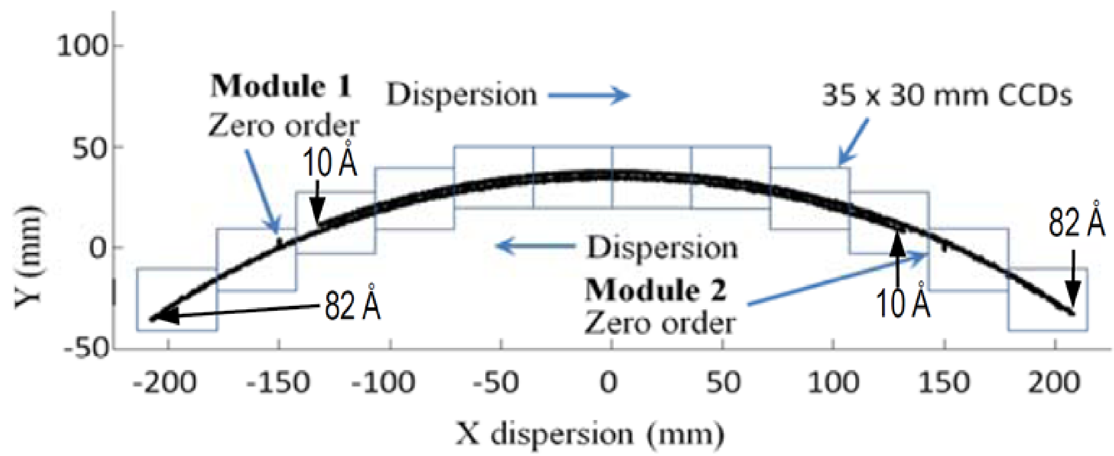


Figure 11: A raytrace of the spectra is shown overlaid on the proposed CCD array. Two arcs, one from each module, disperse in opposite directions. This allows for spectral redundancy.

3. CONCLUSION

Many developments have been made in the last decade during the *Constellation-X*, and subsequently, IXO programs. This development has taken place in optics, gratings, and detectors to support the scientific demands of this major observatory. However, much of this science can still be achieved in a smaller, more cost effective, dedicated instrument onboard an Explorer mission. One such mission, WHIMex, takes the developments made in optics and off-plane grating spectroscopy and applies them to a spectrometer capable of detecting the bulk of normal matter in the universe. Applications such as this will be necessary in the foreseeable future to circumvent what appears to be a likely void in future astronomical X-ray observations.

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