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Invited Paper

A high resolution X-ray spectrometer utilizing Kirkpatrick-Baez optics and off-plane gratings

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ABSTRACT

We present the design of a high resolution X-ray spectrometer for space based X-ray studies. This novel design utilizes a Kirkpatrick-Baez geometry with an off-plane grating as the secondary optic. This design has been proposed to NASA for flight onboard a suborbital rocket. The approach is low cost, low risk and has applications for future orbital missions.

Keywords: X-ray optics, diffraction gratings, CCDs, suborbital rockets

1. HIGH RESOLUTION X-RAY SPECTROMETER

1.1 X-ray optics

An inexpensive and readily available alternative to a slumped glass Wolter telescope is a Kirkpatrick-Baez (KB) configuration[1, 2]. This configuration has the primary and secondary optics in orthogonal planes as shown in figure 1. The optics can be arrayed to increase collecting area. In a KB optical system the mirrors can be surfaces of translation instead of surfaces of rotation. Thus, KB optics are relatively inexpensive because their figure can be met through mechanical confinement as opposed to slumping onto high precision mandrels. Alternatively, the slumping method can also be used, at a lower cost to Wolter arrays, given that the number of required mandrels is smaller. KB optics have been used successfully on sounding rockets for years. Gorenstein et al.[3] obtained 250 cm^2 at 44 Å and 150 cm at 10 Å using 14 plates measuring 51x19.7 cm with a 0.3–2.8° graze angle and a focus of a few arcminutes.

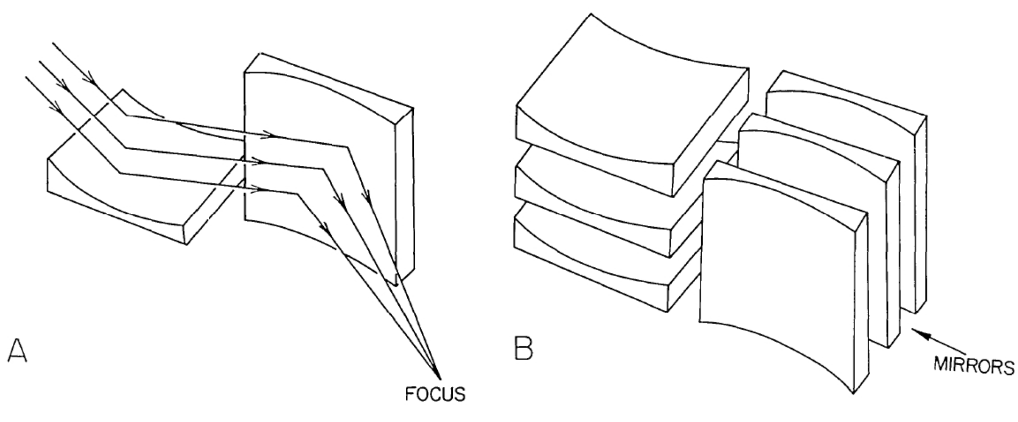

Figure 1: The Kirkpatrick-Baez configuration[1]. On the left, two orthogonal surfaces of translation create a point focus. On the right, these surfaces can be arrayed to increase collecting area.

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For dispersive spectroscopy, the optical focus is only important in one dimension, the dispersion direction. This means that we do not require a complete KB system, just the primary optic which produces a line focus. We then use gratings as a "secondary" and disperse the line focus into a spectrum. This hybrid KB system is modeled in figure 2. The figure depicts a primary optical module on the left side of this model and a grating module on the right side. A closer look at the configuration of the optics is shown in figure 3. The optics module consists of 27 individual optics measuring 200 mm x 100 mm x 0.3 mm each. The graze angle ranges from ~0.6–1.4° and the surfaces will be coated with gold. This results in an effective collecting area of > 67 cm^2 over the bandpass per module. The required shape of the surfaces was calculated to be spherical cylinders with radii of curvature from 239–665 m to form a 3 m focus. The figure shows only rays in a single plane converging to a focus. In a collimated beam, the focus would be a line orthogonal to the page. In a complete system, gratings would be placed in the plane of the page, orthogonal to the optics, thus dispersing the focal line along the plane of the page. The rocket payload will incorporate three optic modules for a total effective collecting area of >200 cm^2 over the bandpass.

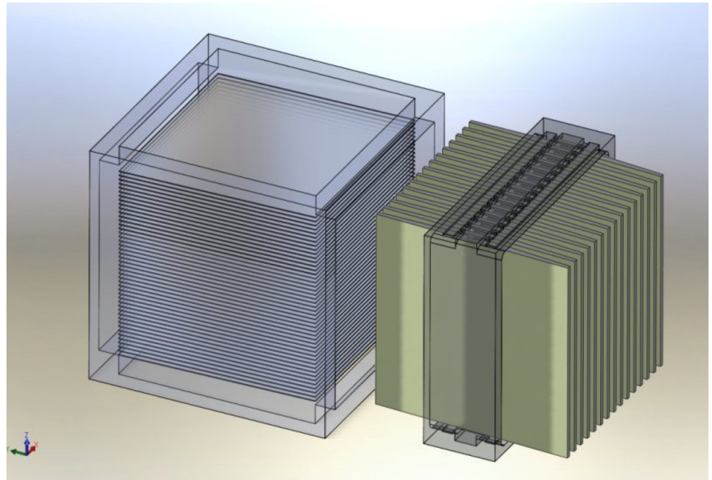

Figure 2: KB system for the proposed sounding rocket payload. The primary array, consisting of spherical cylinders, is shown on the left with the array of off-plane gratings on the right.

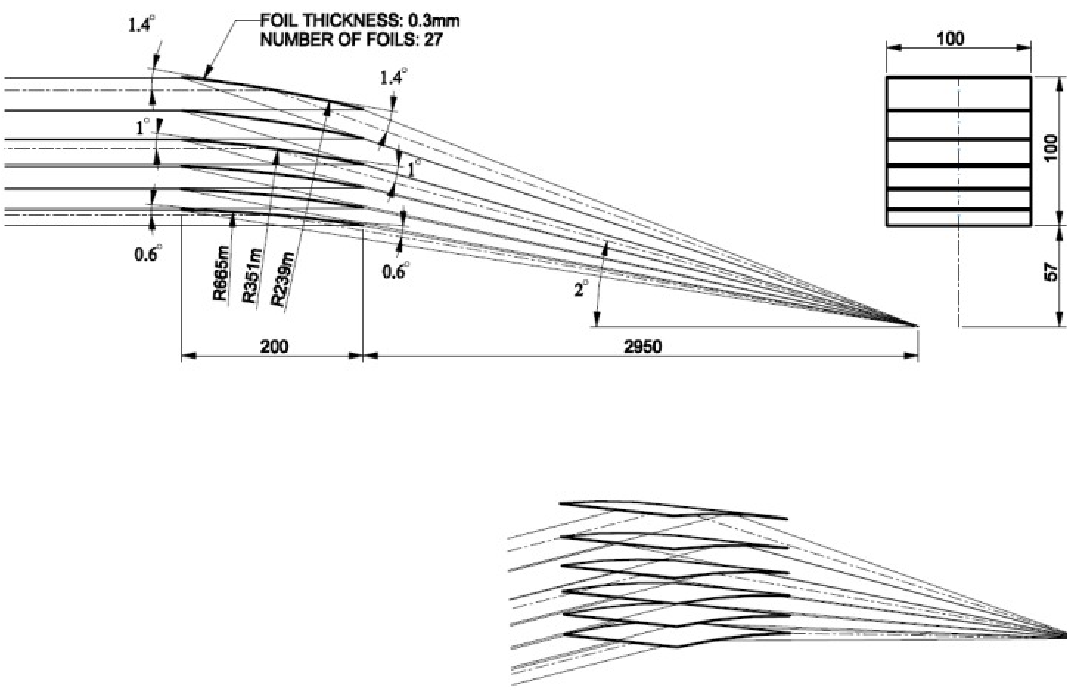

Figure 3: Configuration of the primary optics. Each array will consist of 27 foils measuring 200 × 100 × 0.3 mm. The graze angle will vary over the array from 0.6-1.4°. The radii of curvature of the optics range from 239-665 m for a 3 m focus.

The optics will be procured from Rigaku Innovative Technologies Europe (RITE; formerly Reflex). This company has a professional relationship with the Czech Technical University (CTU), the institute of Co-Investigator Dr. Rene Hudec[4, 5, 6]. RITE has extensive experience in producing multi-foil optics (MFO). An example of two complete KB systems built by RITE and similar to the one proposed here are shown in figure 4. The focus on the right side of this figure came from the system in the middle which consists of 20 gold coated, ellipsoidal surfaces in both the primary and secondary optics. RITE has also obtained excellent quality line foci. Figure 5 shows a test setup and results for a single component KB configuration. The optic is a 300 × 100 × 0.3 mm parabola of translation with a focal length of 1.2 m. The line focus is <14". Using requirements and definitions for the rocket, provided by Dr. McEntaffer, RITE has developed the optical design shown in figure 3 and quoted the rocket optics as obtaining 15" line focus per module on a best effort basis.

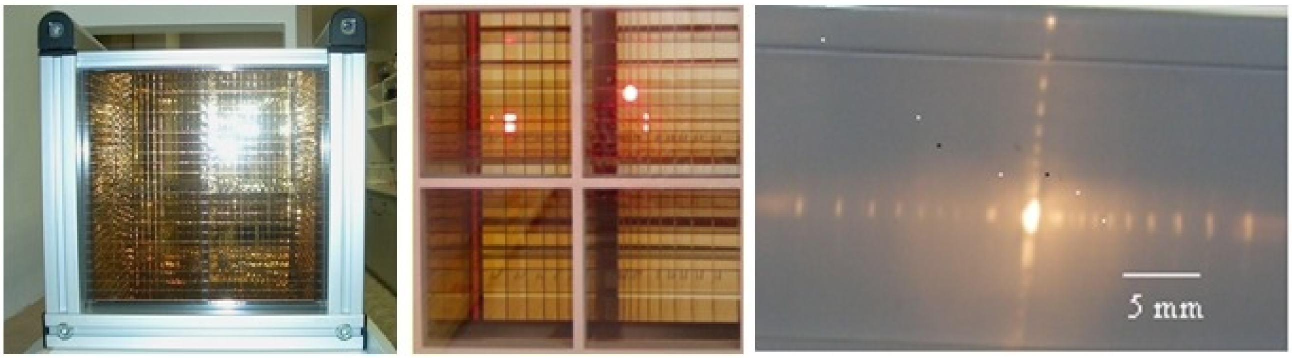

Figure 4: Examples of MFO KB systems built by RITE. The focus on the right was formed from the 40 element KB system shown in the center picture.

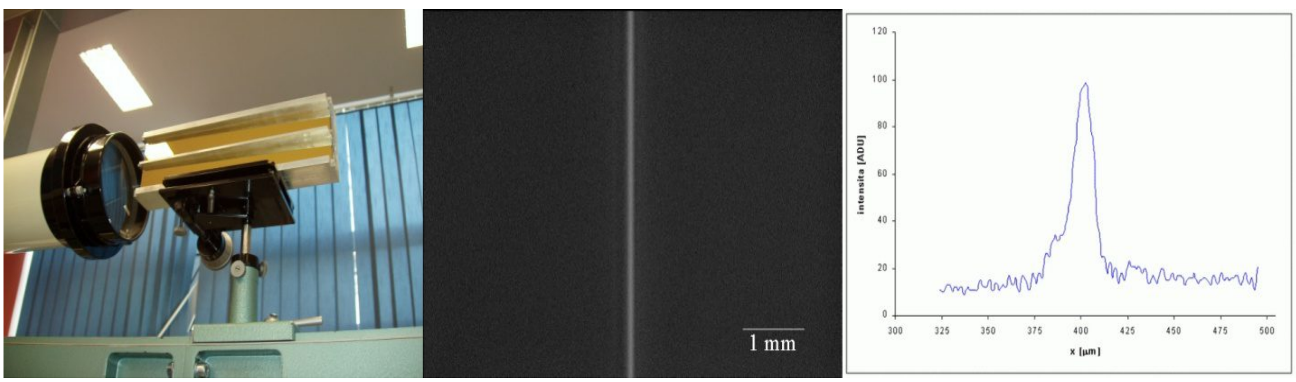

Figure 5: Optical test of a single KB optic similar to those used for the rocket payload. The line focus is shown at the center. The beam profile is shown to the right with a FWHM <14".

1.2 Off-plane reflection grating array

In the off-plane mount, incoming light approaches the grating quasi-parallel to the groove direction and is either specularly reflected into zero order or disperses into a cone of light with dispersion direction orthogonal to the groove direction as shown in figure 6[7]. The typical grating equation still applies, but with an added factor of the sine of the groove incidence angle, γ, where γ is the quadrature sum of the graze angle and the angle that produces α. Just like with X-ray optics, X-ray gratings can be arrayed as well as shown on the right of figure 6. To maintain a constant graze angle over the grating array, the gratings are fanned. This overlaps the individual grating spectra at the focal plane. If the planes of the gratings were projected onto the focal plane, they would form a line that bisects and is orthogonal to the line connecting the telescope focus and zero order. This projection would also be coincident with a diameter of the circle that defines the arc of diffraction. To maintain the focus, the grooves must not be parallel, but radial instead. If projected to the focal plane, the grooves would emanate from a point. This maintains a constant α for the incoming light

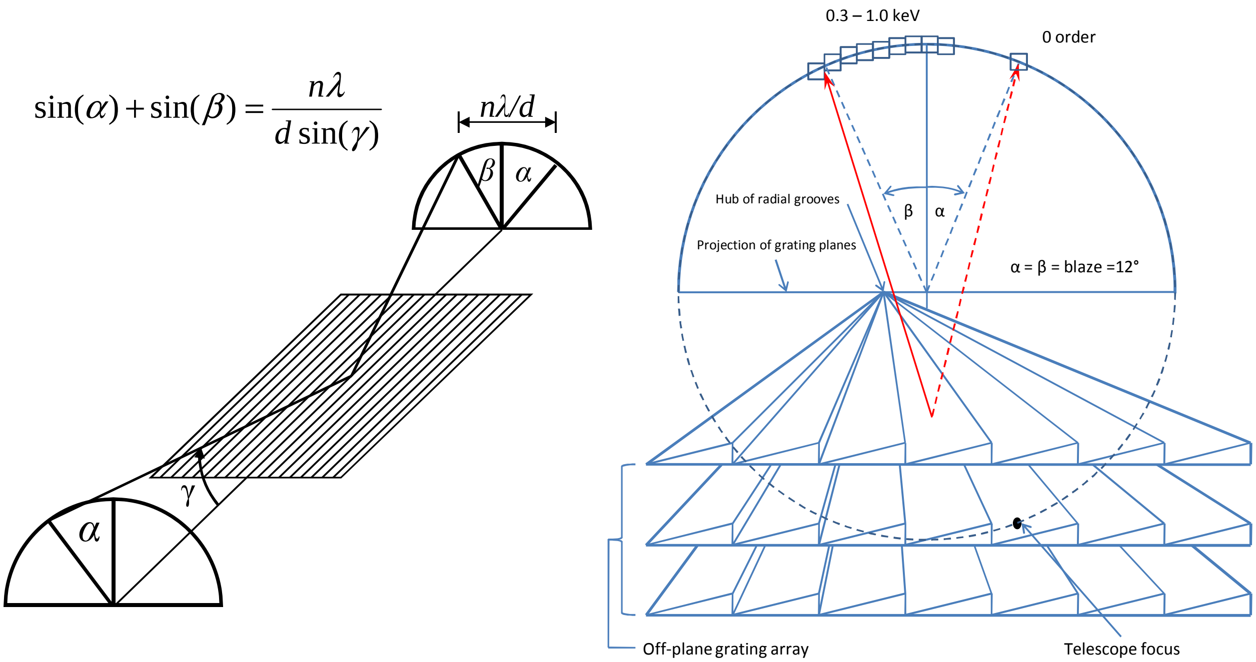

Figure 6: Geometry of the off-plane grating mount. The schematic on the left depicts an incoming ray and the resulting arc of dispersion at the focal plane which follows the given grating equation. The schematic on the right displays the concepts of arrayed gratings, blazed grooves, radial groove profiles, and the arc of diffraction at the focal plane.

and therefore a constant β for a given wavelength, thus avoiding any aberration from the gratings. Finally, the grooves of the grating can be etched or "blazed" to produce individual facets on each groove surface which preferentially disperses light onto one side of zero order thus increasing efficiency in only plus or minus orders and decreasing the size of the CCD array. A grating array constructed in this manner will provide high throughput while maintaining the high resolution of the telescope optics. High groove density will lead to the dispersion that is necessary for high spectral resolution.

Off-plane grating arrays have flown previously on sounding rockets. The Cygnus X-ray Emission Spectroscopic Survey (CyXESS; rocket flight Cash 36.224) utilized an off-plane reflection grating array for observation of the Cygnus Loop supernova remnant at soft X-ray energies (< 0.3 keV)[8, 9]. The spectrum obtained is shown in figure 7. The results of the data analysis show that the soft X-ray flux of the Cygnus Loop is most likely dominated by an equilibrium plasma at a temperature of log(T) = 6.2 with a depletion in Si. The CyXESS payload increased the technology readiness level (TRL) for off-plane grating arrays in future NASA missions, but the gratings themselves were still far off from what will be proposed to fly on the X-ray Grating Spectrometer (XGS) onboard the International X-ray Observatory (*IXO*). In order to address the needs for the XGS, the new grating array described here will be used to nearly duplicate a design proposed for *IXO* and therefore significantly increase the TRL for this major NASA mission.

This proposed rocket payload will use gratings that are nearly identical to the proposed *IXO* gratings and therefore test the current state-of-the-art in this field. They will be the same in terms of the groove density (5500 grooves/mm) optical quality of the surface (λ/4), design of the substrate, the general groove profile (radial, blazed), and the mounting scheme. The only ways in which they will differ is that the rocket grating substrates will be made from 7075 Al instead of Be (to save cost since there is no weight restriction) and the groove profile will converge for a 3 m telescope beam instead of a

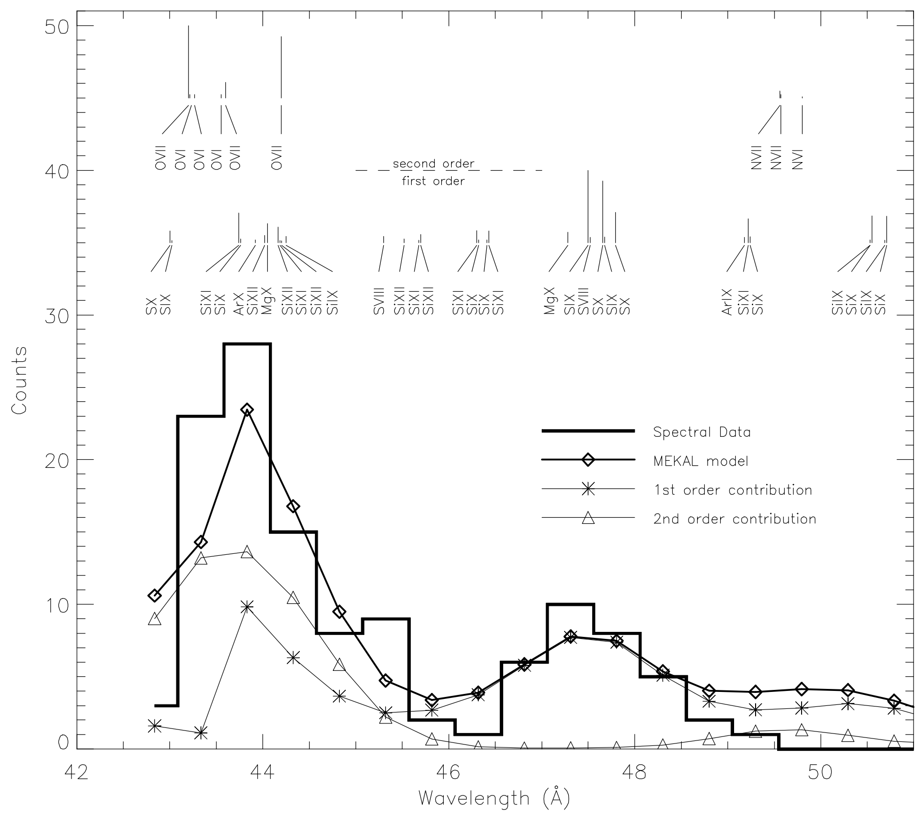

Figure 7: Spectrum obtained from the CyXESS sounding rocket experiment. The best fit spectrum is an equilibrium plasma with a Si depletion.

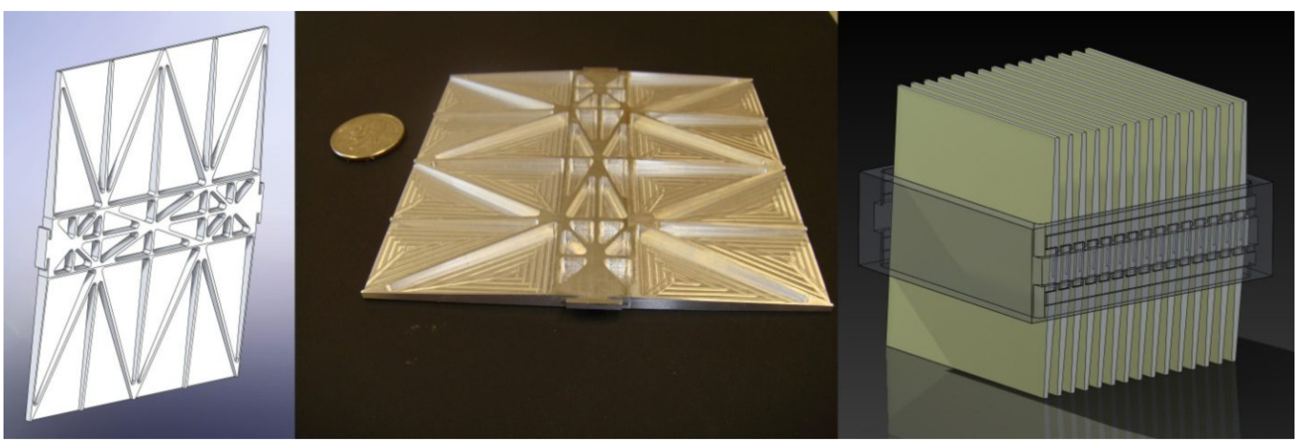

Figure 8: Rocket grating design. The model on the left shows the lightweighted back of a grating. The picture in the middle is the first substrate machined from Al. The model on the right is a full, aligned module of gratings.

20 m focal length. The efficiency requirements are the same and resolution scales with focal length accordingly. A design overview for the rocket gratings is shown in figure 8. The model on the left of this figure shows the backside of an individual grating. Fifteen of these gratings will be arrayed into a single module as shown on the right of this figure. Each grating will be individually aligned. Then, small tabs on each side of the grating are epoxied to the module mount, thus providing the necessary geometry. One of these modules will serve as the "secondary" to each of the telescope

modules described above for a total of 3 grating modules. Production of the Al substrates has already begun and a picture of the first substrate is shown in the middle of this figure. Completed substrates will be sent to the grating manufacturer, Horiba Jobin-Yvon where they will be coated with Ni, polished to figure, and have a grating replicated onto the surface. This is typically performed by applying a thin layer of epoxy onto the optical surface of the grating and pressing a grating submaster onto the surface. The cured epoxy will then have the desired groove profile and will subsequently be coated with a reflective layer such as Au or Ni.

1.3 CCD detectors

X-ray CCDs are workhorse detectors for imaging spectroscopy. For the proposed payload, three X-ray CCD cameras will be used to readout the 3 different telescope/grating arrays. The CCD arrays required to readout the gratings are challenging, even for a rocket experiment, due to the large dispersion, and hence large array size. The requirements of each CCD are as follows: 1) Imaging readout, thus a frame transfer region is needed; 2) Back-illumination for enhanced soft X-ray efficiency, 3) Relatively high frame rate, to reduce photon pileup; 4) Energy range from 300 eV to 1500 eV; 4) Energy resolution of better than 200 eV FWHM for order separation; 5) Spatial resolution of < 30 μm. Given the soft X-ray energy range required, the CCD must be a backside illuminated (BI) device with a depletion depth of at least 10 μm. This technology has been flown in the past on *Chandra* (2 BI CCDs) and *XMM* (18 BI CCDs). However, additional technology developments are being performed as part of the *IXO* studies (and other missions) to enhance the detection efficiency, radiation hardness, and optical light rejection of these devices.

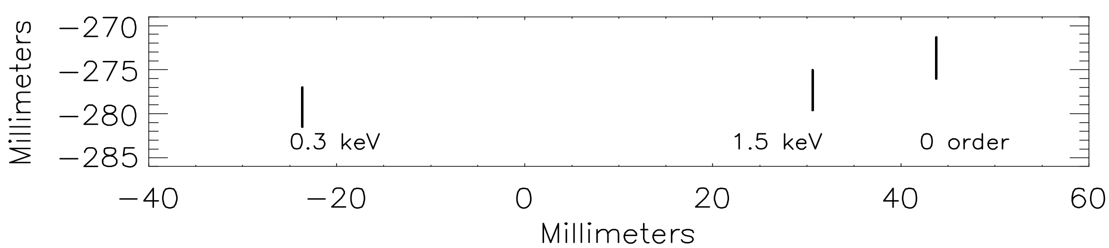

Figure 9: Raytrace of the optics and gratings at the focal plane.

One of the key issues for this sounding rocket payload is the relatively large focal plane size required to cover the grating readout. While there are several solutions that can be adopted for the application, we propose to utilize a single CCD204 from e2v Technologies for each focal plane to cover the 0.3-1.5 keV dispersion. In addition, we will utilize a small CCD to capture the zero order light and provide a wavelength reference. A raytrace of the rocket showing the spectrum at the focal plane is shown in figure 9. As seen from this raytrace, a 50 mm device will just cover the 0.3-1.5 keV bandpass. Figure 10 shows the CCD204 back illuminated device that will be used to capture this spectrum. This CCD is currently being evaluated by ESA as the radiation damage test vehicle for use in the optical camera for the ESA *Euclid* merged mission concept. The group at the Open University is working closely on this project and can make use of the synergies between *Euclid* and the requirements for this rocket proposal.

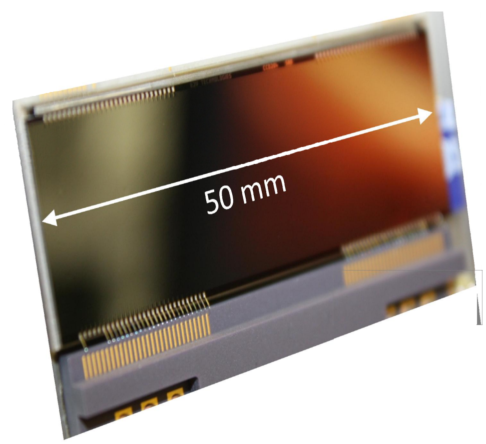

Figure 10: An e2v Technologies CCD204

The three CCDs will be cooled to approximately -50° C using a Peltier cooler, which will be heatsunk to the rocket structure. For laboratory testing we will use commercially available CCD readout electronics, but will develop dedicated control and digital processing units for this application and to prove key technologies for *IXO*, namely low noise analog electronics and ADC ASICs, which will be obtained free-of-charge from the UK Rutherford Appleton Laboratory. Their Mark 5 CDS/ADC ASICs have been qualified and flown in the imaging cameras for the *Solar Dynamic Observatory*. We intend to use the later Mark 7 designs for these cameras. X-ray CCDs in photon counting mode produce images with mainly background, interspersed by signal flashes from the X-ray photons. In addition we will build X-ray event detection units, using the Analog Devices DSP family, which have been qualified in the UK for the *Beagle-2* mission. The event detection units will strip X-ray photon data from the raw image data stream.

The resulting events will be passed on to the telemetry system of the rocket for download. The expected countrate of the source plus background from each of the three modules is 100-200 counts/second (depending on which model is supported). This amounts to a telemetry requirement of ~50 kbps. Previous experience with sounding rocket telemetry combined with recent discussions with NSROC telemetry engineers shows that a dedicated science telemetry stack is capable of synchronously sampling the payload at 100 kHz allowing for a telemetry rate of 9.6 Mbps, easily reading out the CCDs.

2. ROCKET PAYLOAD

Figure 11 shows an engineering diagram of the nearly complete sounding rocket payload. It is an aft facing payload with a shutter door at the aft end. Three telescope modules will be positioned as shown, just inside the shutter door. The grating modules will be packed into assemblies immediately after the telescopes. Both the optics modules and the grating modules will be mounted to a common structural mounting plate within the payload. This plate will also house the ST5000 star tracker camera (oriented along the roll axis).

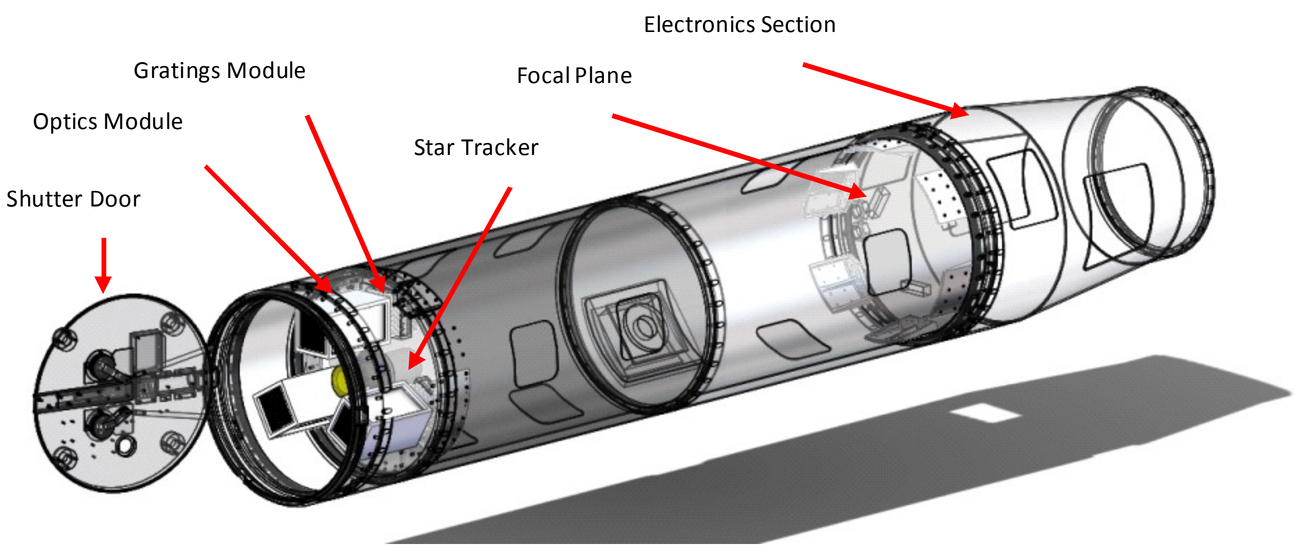

Figure 11: Engineering model of the rocket payload from the aft facing shutter door to the electronics/telemetry system. The optics and gratings modules are mounted to a plate cantilevered from the focal plane.

Experience with these star trackers combined with recent flight results show that they (ST5000 camera built at the University of Wisconsin with the NSROC Celestial Attitude Control System, CACS) are capable of subarcsecond pointing (~0.6 ″ RMS over a flight). An interior support structure cantilevers the optics assembly off of the detector bulkhead (labeled Focal Plane in the figure) to negate any influence from the rocket skins. A nearly identical support structure was flown on flight Cash 36.224. This interior support structure is attached to the bulkhead and the optics/grating mount plate using robust mounting feet. A pump-out port is located on the side of the skin. A turbo pump is attached to this port to evacuate the payload (< 10^{-5} Torr). Due to contamination concerns, the payload will be evacuated or backfilled with ultra high purity N_2 at all times. Finally, all of the CCD detector electronics, cryogenics and telemetry interfacing reside in the electronics transition section.

Even before telescope modules are assembled or grating arrays populated, we will be able to work on system integration issues. First, a full system raytrace will be developed complete with tolerancing to understand the alignment issues that we will have not only between components but within components as well. Furthermore, while awaiting fabrication of the various systems, calibration issues can be studied in real life utilizing *IXO* development products such as gratings, test CCDs and optics.

During final assembly, one of the first steps in system integration will be to align the three telescope assemblies within the rocket. Currently, this can be easily done to 30″, but during this program work will be done to achieve < 10″ alignment. The final telescope assembly will include reference flats for accurate alignment of the gratings and star tracker. However, the telescope alignment is not critically important; the grating arrays can be used to steer the light path onto the CCDs. Small tweaks to the attitude of the gratings will be able to align the beam to the CCDs with a negligible effect on throughput, if any. Furthermore, this allows independence from any imperfections or tolerance stack-up in the support structures.

3. EXPECTED PERFORMANCE

Figure 12 displays a group of plots that describe the expected performance from the rocket payload. First, the plot on the upper left shows the CCD QE and filter efficiency. The black line shows the overall efficiency of a backside illuminated CCD device incorporating an optical blocking filter made from 26 nm of MgF_2 and 75 nm of Al. Next, the plot on the upper right shows the theoretical diffraction efficiency of the proposed gratings in orders 1–5. The black line gives the sum of orders. It is important to note that this efficiency includes the reflection efficiency of Au at 2.7° graze over the bandpass. In practice, these orders will overlap at the CCDs. The energy resolution of the photon counting CCDs will provide the order separation. The top curve on the bottom left shows the reflection efficiency of the optical modules assuming an average graze angle of 1° and Au coating. The bottom curve shows the combined efficiencies of the optics, gratings and CCDs. Finally, the plot on the bottom right displays the total effective area of the three modules on the rocket. The ~90 cm^2 contained within this rocket payload will provide nearly a tenth of the effective area of the *IXO* XGS for 0.05% of the budget.

The theoretical resolution for the rocket gratings, given their profiles, is displayed in figure 13 for multiple orders depending on wavelength. The lowest wavelength lines will have their highest efficiency (see figure 12) in fourth order (blue line) or third order (green line) while longer wavelength lines are most efficient in second (orange line) and first order (red line). In this way, we will achieve high resolution concurrently with high throughput. Also, this provides for a more constant resolution across the bandpass given that resolution scales with order number while $\Delta\lambda$ remains constant (grating dispersion remains constant with wavelength). The payload will acquire a resolution of ~ 200–300 over the bandpass. Resolution of this level is necessary to perform plasma diagnostics such as those found in the He-like triplet of O VII. The ratio of forbidden line flux to the intercombination line flux is an important density diagnostic. Furthermore, the O VII to O VIII flux ratio determines temperature and ionization state. Figure 14 displays the expected resolution of the rocket payload as it pertains to the O VII triplet. At this resolution the resonance (21.6 Å), intercombination (21.8 Å), and forbidden (22.1 Å) lines are easily distinguished.

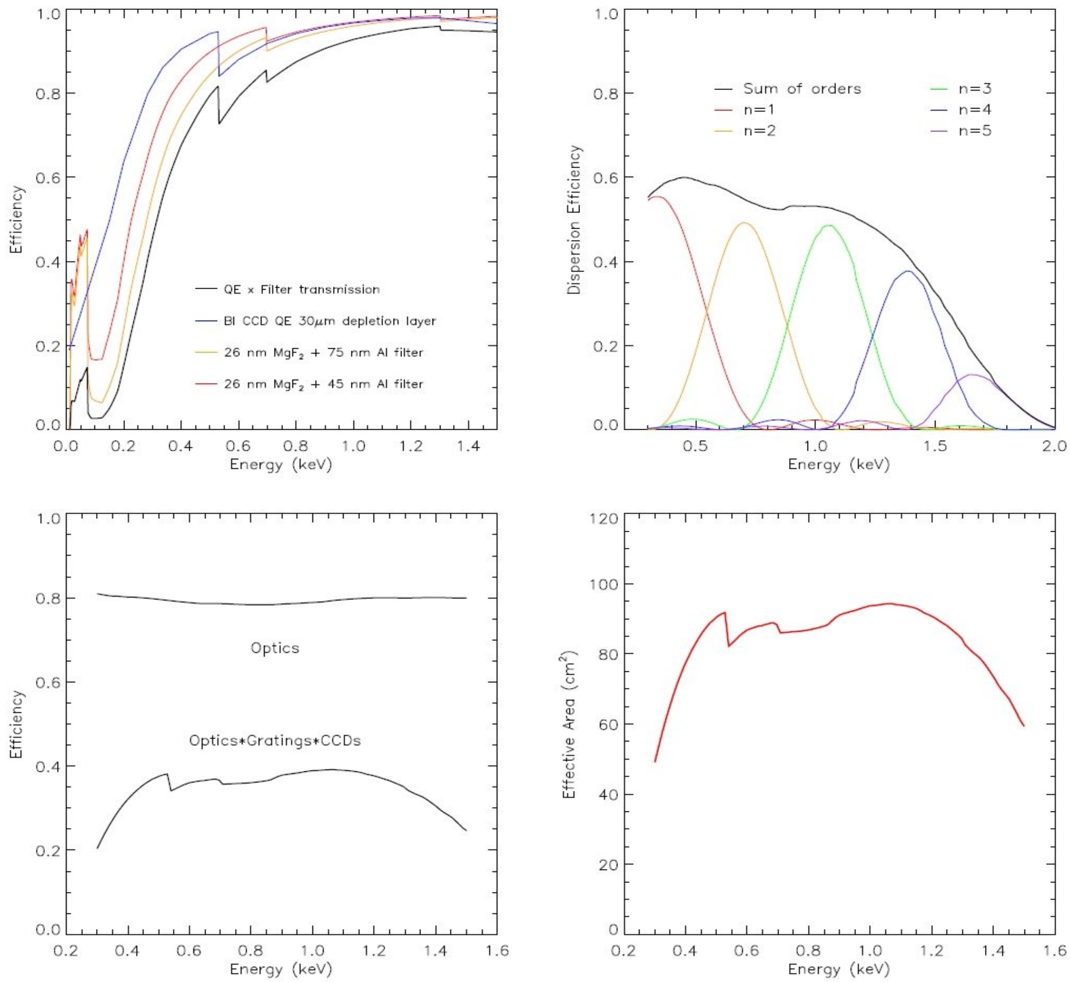

Figure 12: Expected performance of the rocket payload. CCD QE is given in the upper left. The grating efficiency at various orders is on the upper right with reflection of Au at 2.7° folded in. The lower left shows the overall payload efficiency while the lower right gives the effective area of the entire payload, all three modules.

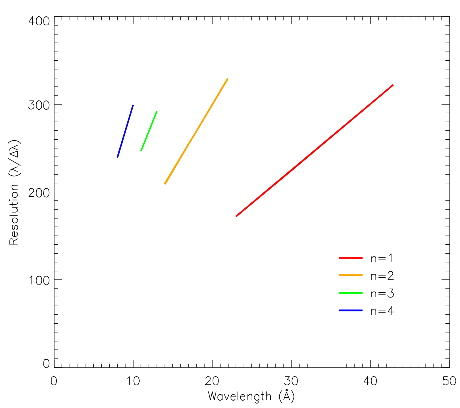

Figure 13: Rocket payload spectral resolution.

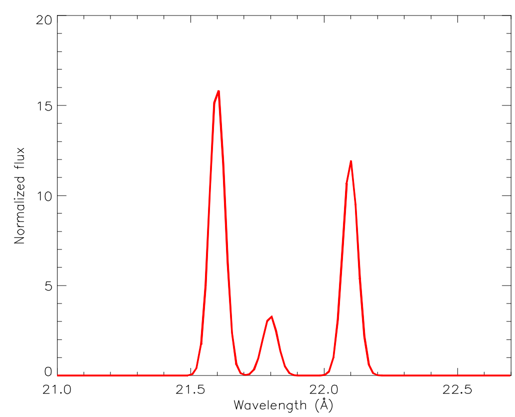

Figure 14: Simulation of the He-like triplet of OVII as observed with the rocket payload.

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