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The simulated spectrum of the OGRE X-ray EM-CCD camera system

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ABSTRACT: The X-ray astronomical telescopes in use today, such as Chandra and XMM-Newton, use X-ray grating spectrometers to probe the high energy physics of the Universe. These instruments typically use reflective optics for focussing onto gratings that disperse incident X-rays across a detector, often a Charge-Coupled Device (CCD). The X-ray energy is determined from the position that it was detected on the CCD. Improved technology for the next generation of X-ray grating spectrometers has been developed and will be tested on a sounding rocket experiment known as the Off-plane Grating Rocket Experiment (OGRE).

OGRE aims to capture the highest resolution soft X-ray spectrum of Capella, a well-known astronomical X-ray source, during an observation period lasting between 3 and 6 minutes whilst proving the performance and suitability of three key components. These three components consist of a telescope made from silicon mirrors, gold coated silicon X-ray diffraction gratings and a camera that comprises of four Electron-Multiplying (EM)-CCDs that will be arranged to observe the soft X-rays dispersed by the gratings.

EM-CCDs have an architecture similar to standard CCDs, with the addition of an EM gain register where the electron signal is amplified so that the effective signal-to-noise ratio of the imager is improved. The devices also have incredibly favourable Quantum Efficiency values for detecting soft X-ray photons. On OGRE, this improved detector performance allows for easier identification of low energy X-rays and fast readouts due to the amplified signal charge making readout noise almost negligible.

A simulation that applies the OGRE instrument performance to the Capella soft X-ray spectrum has been developed that allows the distribution of X-rays onto the EM-CCDs to be predicted. A proposed optical model is also discussed which would enable the missions minimum success criteria's photon count requirement to have a high chance of being met with the shortest possible observation time. These results are compared to a Chandra observation to show the overall effectiveness of the new technologies. The current optical module is shown to narrowly meet the minimum success conditions whilst the proposed model comfortably demonstrates the effectiveness of the technologies if a larger effective area is provided.

KEYWORDS: Photon detectors for UV, visible and IR photons (solid-state) (PIN diodes, APDs, Si-PMTs, G-APDs, CCDs, EBCCDs, EMCCDs etc); Spectrometers; X-ray detectors

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1 Introduction

X-ray astronomy is a difficult field requiring alternative approaches to telescopes imaging elsewhere in the electromagnetic spectrum. Synchrotron/bremsstrahlung radiation from distant galaxy clusters is invaluable to some studies whilst monitoring the thermal properties of stars as near as our own are of interest to others. With the Earth's atmosphere absorbing the incoming X-rays, ground observations are impossible meaning space-based telescopes such as XMM-Newton, Chandra, and more recently the Soft X-ray Telescope (SXT) instrument on ASTROSAT, are required. Whilst some instruments focus on generating images for observation, others focus on splitting the photons into a spectrum to better determine the properties of their source.

The Off-plane Grating Rocket Experiment, or OGRE, is one such telescope which will build on the latest instrument technologies to demonstrate their performance for future large scale projects. OGRE is a sounding rocket experiment designed to acquire the highest resolution spectrum of Capella to date with a launch date of 2019. In order to determine the model the performance of OGRE, an end to end simulation was developed to see how each of the instrumentation components contribute to the collected spectrum.

Figure 1. The Capella spectrum extracted from the Chandra data using each energy bins effective area and the 84597 second exposure.

1.1 Previous Missions

Telescopes such as XMM-Newton and Chandra utilise two sets of nested glass mirrors in a formation known as a Wolter-1 telescope [1]. The photons are then incident on a diffraction grating which disperses the X-rays according to their energy. A position sensitive detector is used to observe the photons, and therefore infer the energy spectrum. Chandra has observed the OGRE’s target, Capella, and the data from this observation has been used as input to the simulation presented here (figure 1) and used as a direct comparison for the performance of OGRE.

1.2 The OGRE project

As well as acquiring the highest resolution spectrum of Capella OGRE also aims to improve the Technology Readiness Level (TRL) of the payload’s three major components: the silicon mirror optics system, the off-plane diffraction gratings, and an EM-CCD camera (figure 2). Each of these components have been tested and validated in labs meaning they are currently at a NASA TRL of 4. If a spectrum in the soft X-ray energy range of 600 eV to 1200 eV is successfully obtained during OGRE’s 3-6 minute observation time, the components will have been shown as flight qualified through demonstration and, for sounding rocket use, see a TRL increase to 8.

2 Silicon optics

In order to effectively collect photons from Capella, a Wolter-1 telescope design, similar to that seen in Chandra, will be utilised on OGRE. The parabolic and hyperbolic mirrors will be made of silicon to allow for high reflectivities in the soft X-ray energy range as well as reducing the mass of the optical system relative to a typical glass optic system. The silicon mirrors will be assembled using

Figure 2. The OGRE instrument light path showing the silicon mirrors, diffraction gratings and the EM-CCD camera that make up its three main components. Note: not to scale.

Figure 3. CAD rendering of one of the three OGRE mirror modules. The two 30° segments for each mirror type are different and partnered to make a 60° module. Figure courtesy of Ryan McClelland (NASA GSFC/SGT Inc.).

a meta-shell system being developed by the NASA Goddard Flight Center [2]. This new method of mirror assembly allows larger areas to be covered by a single unit whereas other telescopes have relied on many narrow wedges with bulky casings which limit the usable observation area.

2.1 Optical designs

The OGRE system will feature three mirror modules, each covering a 60° azimuth. A test module has been developed to check the structural stability of the meta-shell assembly. This design features 8 mirror shells with an inner radius of 165.03 mm and an outer radius of 180.94 mm for the parabolic mirrors and an inner radius of 161.73 mm and an outer radius of 179.54 mm for the hyperbolic mirrors (figure 3). Assuming all reflected light is incident off the parabolic mirrors and successfully reflected onto the hyperbolic mirrors, the total aperture area of 0.0129 m^2 .

With the structural tests being successful it may be possible to add additional mirror layers to each module and thus increase the collection area of the telescope. A proposed model was created after the initial simulation and intends to fulfil the mission's minimum success criteria of a spectral line containing at least 25 photons in the minimum possible observing time. Obtaining a larger photon count could allow for narrower binning in the spectrum assuming the accuracy of the read out position of a photons incidence on a detector is sufficiently high. The proposed system therefore

Figure 4. The reflectivity of silicon over the OGRE soft X-ray energy range when photons are incident with a graze angle of 1° .

Table 1. The effective areas of the discussed projects' optical arrays at 1000 eV.

Optical Model	Effective area of the optics at 1000 eV (m ²)
8-shell mechanical	0.01019
12-shell proposed	0.01593
Chandra	0.04 [3]

features 12 shells with the additional layers being added to the outside of the original 8-shell system and covering the 60° azimuth. This gives an exposed optical area of 0.0202 m².

2.2 Effective areas

As the reflectivity of the mirrors is dependent on the photon energy and the incidence angle an effective area is often given when discussing the performance of a telescope. The geometric telescope aperture is therefore multiplied by the squared reflectivity of the mirror material to take the two mirror system into account thus giving its effective area. Whilst it's common practice to coat the mirrors to better reflect the desired energy, e.g. iridium coatings for broader X-ray observations, the OGRE energy range will benefit more from using plain silicon mirrors. Taking the reflectivity of silicon (figure 4) gives the effective areas seen in table 1.

3 The off-plane diffraction gratings

Diffraction gratings provide a means of obtaining high energy resolution with spectrometers by dispersing the X-rays across a position sensitive detector. Optimisation of soft X-ray diffraction

Figure 5. The profile of the off-plane diffraction gratings. The triangular grooves can be clearly seen which will allow the preferential distribution of the X-rays.

gratings has been a subject of development for a range of applications, from synchrotron to space instrumentation applications. The gratings for OGRE are being developed at Penn State University specifically for optimum performance in the soft X-ray range. The placement of the gratings in the off-plane geometry allows for better resolving power at higher orders due to a drastic reduction in vignetting [4]. The design of the groove profile allows for them to be fully illuminated in this orientation meaning groove shadowing doesn't occur and therefore a higher efficiency is obtained.

The gratings will feature a blazed profile (figure 5). By etching triangular grooves into the surface the photons are preferentially distributed to one side of the zero order. If this is done effectively the area required to collect all diffracted light is reduced to half of that of a non-blazed grating. The gratings will also be placed in a Littrow configuration. By applying a yaw to the angle the gratings are mounted at the photons can be preferentially diffracted to certain orders.

The combination of these design choices (blazed profile, off-plane orientation, Littrow configuration) implemented into the gratings, optimise the gratings by maximising diffraction efficiency whilst minimising the focal plane area required. The grating design will be optimised for the OGRE application, but the manufacturing technology will be proven for future applications.

3.1 Grating efficiency

The gratings to be used in the OGRE payload are made of fused silica with a gold coating [5]. Photons will be incident upon the gratings which have a blaze angle of 29.5° with a yaw of 0.85° to implement the Littrow configuration. A grating density of 6250 grooves/mm will be used. Simulations of the grating setup (using PCGrate-SX V6.1) gives the grating efficiency seen in figure 6. For the sake of this simulation it has been assumed that the focal plane and the arrangement of the gratings have been designed to allow for all orders within the OGRE range to be incident upon the detectors so this may be an overestimation.

4 Optical blocking filter

The design of the OGRE payload means that optical light will be incident upon the detectors as well as the X-ray photons. For this reason an optical blocking filter will need to be used to prevent optical and ultraviolet photons from reaching the detector whilst allowing a good transmission of X-ray photons. The final filter format is to be confirmed, but the modelling presented here has adopted a worst-case design that was originally proposed for the CLASS instrument on Chandrayaan-2, 0.4 μm of polyimide and 0.2 μm of aluminium [6]. The aluminium is an efficient optical filter, whilst the polyimide is opaque in the ultraviolet range. The modelled X-ray transmission of this filter

Figure 6. The total grating efficiency over a broad energy range (black line) which covers the OGRE energy range (red line). This is the sum of the individual order efficiencies (greens dashed is first order, purple is second order, yellow is third order, orange is fourth order and blue is fifth order).

configuration is shown in figure 7. A reduced transmission is observed at the lower end of the OGRE energy range therefore alternative filter configurations will be investigated for OGRE, but this model indicates the worst-case performance.

5 The EM-CCD quantum efficiency

OGRE will utilise an EM-CCD (Electron Multiplying CCD) camera which features four CCD207-40s. The image section is comprised of 1600×1600 pixels each of which is $16\mu\text{m} \times 16\mu\text{m}$ (figure 8). The advantage of using EM-CCDs rather than standard CCD or CMOS devices is the insertion of a 536 element, multiplication register before the readout node. There is a chance impact ionisation occurs in each element which will increase the signal within a pixels charge packet. The more electrons initially in the charge packet, the higher the chance that the signal is increased. By repeating this many times a packet which was initially small can become large. The readout register will add noise to every pixel that is read out however the amount added is independent of the charge within each pixel. As the charge packet is now much larger than the smaller readout noise it can be assumed that this noise is negligible [7].

Whilst these devices will be capable of amplifying the signal observed for X-ray photons, the Quantum Efficiency (QE) must also be looked at to see the probability that a photon incident on the device will be detected. The CCD207-40s are uncoated, back-illuminated devices and have enhanced back-surface passivation [9] allowing an improved soft X-ray Quantum Efficiency (QE). Data from an experimental run on a CCD97, an EM device with an identical pixel architecture to the CCD207-40 but a smaller image area, was used in the simulation [10]. The measured data is

Figure 7. Transmissions of the optical blocking filters which could be used in the OGRE instrument.

Figure 8. Schematic of the CCD207-40. The High Responsivity (HR) readout will not be used in OGRE as this allows for standard CCD operation. The Large Signal (LS) readout will be used to allow the gain register to increase the number of electrons in a charge packet [8].

Figure 9. The measured QE of CCD97 (dotted line with data markers) was used to predict the QE over the OGRE energy range (red line).

shown in figure 9, with a spline fit that was used to interpolate the measured QE for intermediate energies. An upper limit of 1 (100% efficient) was applied to the interpolation.

6 Overall effective areas

By taking into account the effectiveness of each component in the OGRE payload the effective area of the instrument for a given photon energy can be calculated. This was done for the 8-shell testing optics modules and the proposed 12-shell optics design as well as the Chandra data to allow for a comparison of how the new technologies perform. When comparing the optical effective areas in table 1 to the overall effective areas of the systems in figure 10, it becomes apparent that the OGRE configuration allows for an improved effective area due to the effectiveness of the grating and the EM-CCDs quantum efficiency.

7 Simulated spectra

To create an input spectrum of Capella, data from Chandra was used. Whilst OGRE aims to measure the highest resolution spectrum of Capella, the current simulation is limited by the energy bin width of the Chandra observation. The data provided the number of source counts and the effective area of each bin which, when combined with the knowledge that the observation time was 84597 s, allows an input flux to be found. Combining this with the calculated effective areas allows a spectrum to be simulated (figure 11).

The resultant spectrum delivers promising results. The largest spectral line at 825 eV corresponds to the Fe-XVII line. As the Fe-XVII line is the most populated in the Chandra data it is a good target for OGRE to achieve observation of a spectral line with more than 25 photons in during

Figure 10. The total instrument effective areas of the 8-shell (red line) and 12-shell (blue line) OGRE optics models and of the Chandra telescope (black line) over the OGRE soft X-ray energy range of 600 eV to 1200 eV.

Figure 11. The time independent spectrum of OGRE for the 8-shell optics system (red line), the 12-shell optics system (blue line), and Chandra.

the observation. The actual Capella observation time OGRE will have is estimated to be between 3 and 6 minutes which gives a minimum required flux of 0.069 to 0.139 photons per second per line. Table 2 shows the simulation outputs for the Fe-XVII fluxes.

These results show that the 8-shell system is likely to meet the required photon count if given a long enough observation time (at least 4 minutes and 20 seconds would make a minimum of 25 photons the most likely result) however some improvements may be needed to ensure success if the minimum observation time of 3 minutes occurs. The 12-shell system would require 2 minutes and 48 seconds to make at least 25 photons the most likely outcome which proves how increasing the collection area can greatly benefit the project.

Table 2. The predicted flux of the OGRE models and Chandra for the most populated spectral line in the OGRE energy range.

Simulation Model	825 eV Fe-XVII spectral line photons (average counts s ⁻¹)
OGRE 8-shell	0.096
OGRE 12-shell	0.149
Chandra	0.065

The largest photon loss comes from the diffraction gratings, however the design of this component may improve before launch due to changes in the groove density, surface area and the applied yaw. The throughput of the optical blocking filter is expected to be improved by adopting a thinner design, allowing for more photons to be detected overall. The other areas of the payload are shown to be highly effective giving close to 100% efficiencies over the OGRE X-ray energy range.

It should also be noted that the energy bins used for this simulation will not necessarily reflect those seen in the final spectrum. The energy resolution of the OGRE camera is under investigation and since the throw from the gratings to the focal plane is fixed, the resolution is primarily dependent on the grating groove density, manufacturing quality, and the detector spatial resolution. The OGRE EM-CCD camera will utilise centroiding to determine the incident X-ray position on the device to a sub-pixel accuracy [11]. The model will continue to be developed to account for the area coverage of the detectors on the focal plane and including energy resolution estimation. The improved energy resolution should allow for separation of multi-peaks in the Capella spectrum, such as the one seen at 724 eV in figure 11.

8 Conclusions

The OGRE spectrum simulation presented here demonstrates that the high throughput design of OGRE will allow it to collect a spectrum with at least 25 photons in a single spectral line. Whilst it has been shown that the 8 shell optic could still meet the mission success criteria it would be better to use a minimum of 12 shells as seen in the proposed model to ensure mission success in the event of a short observation time. With the launch planned for 2019, there is still time for some refinement to the components to further improve the spectrometer throughput and/or resolution.

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