The X-ray Grating Spectroscopy Probe
An APC white paper for the Astro 2020 Decadal Survey

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1 Summary

High resolution spectroscopy conveys dynamical information about processes such as accretion, winds, and rotation and reveals feedback that manifests as turbulence. It allows the separation of multiple velocity components and permits the detection of weaker lines. High-resolution soft X-ray spectroscopy with sufficient resolution and sensitivity has the unique capability to address three critical questions: (1) “How do baryons cycle in and out of galaxies, and what do they do while they are there?” (2) “How do black holes grow, radiate, and influence their surroundings?” (3) “How do rotation and magnetic fields affect stars?”

The Astro2010 Decadal report concluded that conducting revolutionary research on these topics requires spectral resolving powers of R~3000 with effective areas of ~1000 cm² across a wide portion of the X-ray bandpass, capabilities well beyond the existing X-ray instruments on Chandra and XMM-Newton. While micro-calorimeters are being built to address the need for this combination of resolution and effective area at higher energies in the near future (e.g., XRISM, Athena), there is currently no funded mission with instrumentation that can achieve these specifications below ~2 keV where the critical emission and absorption features due to O VII, O VIII, Ne IX, and S XI, for example, are found. An X-ray Grating Spectroscopy Probe (XGS-P) mission utilizing diffraction gratings can access the key low energy X-ray bandpass and provide the performance requirements necessary to address these key science questions.

2 XGS-P Science

2.1 Finding and Characterizing the Missing Baryons

Numerical simulations indicate that accretion shocks and feedback from supernovae and active galactic nuclei (AGN) naturally result in the production of hot gas in galaxy groups and clusters, as well as galactic halos and the Warm-Hot Intergalactic Medium (WHIM) filaments that comprise the cosmic web where the vast majority of baryons and metals at z<1 are predicted to lie [1,2,3,4]. Without the proper instrumentation these components have proven to be notoriously difficult to observe.

Figure 1: Demonstration of using baryon census data to measure the slope of the radial density distribution of galactic halos to beyond the virial radius. The background QSO shines through the haloes of multiple foreground galaxies, imprinting absorption lines from the oxygen gas in each halo along the way (lower inset). These absorption lines appear at each galaxy’s redshift, measuring the amount of gas vs. radius from each galaxy along the line of sight (purple points in upper inset). Data from multiple lines of sight fills in the plot.
At the virial temperature of the hot gas in galaxies, groups and the cosmic web (\(10^{5.5} - 10^{6.8}\) K), nearly all dominant ion transitions occur in the X-ray bandpass. As such, X-ray observations of distant, bright point sources viewed through this intervening gas can uniquely measure the WHIM properties through absorption line spectroscopy. Absorption by O VII, O VIII and other X-ray lines is already detected in the Milky Way halo gas [5,6,7,8] with a column density more than an order of magnitude greater than the lower ionization absorption lines (H I through O VI; [9,10]). However, existing observations lack the sensitivity to determine the fundamental properties of the WHIM in different hosts as well as the relative roles of critical feedback processes.

A direct, unbiased survey of the highly ionized gas in the Universe can be obtained by measuring its X-ray absorption along many lines of sight to bright background AGN. The XGS-P, with R~5000 and an effective area of ~1000 cm\(^2\), achieves the sensitivity needed to conduct such a WHIM census within one year of mission operations, measuring equivalent widths in O VII as low as 1mÅ (see Figure 1).

2.2 Quantifying the Impact of Black Hole Winds on Their Surroundings

To determine how galactic-scale outflows from supermassive black holes influence the structure and evolution of the interstellar medium and beyond, we must identify the launching mechanism(s) of their winds and mass outflow rates by measuring the wind densities, ionization states and velocities. Comparing outflow properties from the launch point (AGN) to downstream (molecular clouds, ISM) is necessary in order to fully understand how such feedback acts on the host galaxy.

At longer wavelengths, ALMA, optical IFUs on ELTs, and JWST will be most sensitive to the large-scale, downstream effects of black hole feedback through observations of dust and cool gas motions. However, these flows must be traced back to their launching points, where they are visible primarily through emission and absorption from dozens of ions at soft X-ray energies superimposed on the AGN spectrum. Disentangling these features, which can vary strongly on timescales of days to months, requires an X-ray grating spectrometer with high spectral resolution and the sensitivity to reveal the velocity distribution, chemical composition, ionization and location of the gas intrinsic to AGN.

Figure 2: The XGS-P enables measurements of the properties of the intrinsic absorbing gas present in roughly half of all AGN. The properties of the various absorption lines and their changes in response to changes in the luminosity of the central X-ray source yield the velocity of the outflowing gas, its chemical composition, ionization, density and distance. From these quantities, we can finally constrain the kinetic power of these outflows and quantify their impact on the evolution of the host galaxy.
By measuring the ionization of the AGN wind and its response to X-ray continuum flux variations, we can deduce the recombination time of the outflowing gas. This breaks the degeneracy between the gas density and distance from the AGN, which scales as the ionization parameter $\xi = L/nr^2$, where $L$ is the measured luminosity of the ionizing source, $n$ is the gas density and $r$ is its distance from the ionizing source. Once the density and outflow velocity of the gas are measured, we can then compute the mass outflow rate and kinetic luminosity of the wind. These data would also reveal the as-yet-unknown wind launching mechanism(s), e.g., radiative or thermal pressure [11].

2.3 Exploring the Formation and Evolution of Stellar Systems
Understanding how magnetic dynamos form coronae over a range of stellar types, ages and rotation speeds requires measuring the thermodynamic properties of hot gas in stellar magnetic structures and shocks. To gain insight into stellar evolution, we must also probe accretion onto young stars and the atmospheric buildup of exoplanets. The key diagnostics of these processes all occur in the soft X-rays, making this prime science for the XGS-P.

X-ray-emitting coronae are manifestations of magnetic dynamos that operate within the stellar convection zone. We can explore the evolution of the magnetic dynamo through measurements of both coronal structure and heating for a rich sample of stars of different ages and types. Coronal properties can be uniquely determined from high-resolution X-ray spectra using emission measure distribution (EMD) analysis, which has so far been applied only to the brightest, most active stellar coronae [12], many in binary systems. The XGS-P can resolve He-like density diagnostics even in the presence of multiple velocity components, as shown in Figure 3 (left). These data will reveal the sizes of coronal structures and any dependencies on stellar age or type [13].

Figure 2: The XGS-P would differentiate between the distinct line signatures produced by accretion shocks near the surface vs. those from coronal emission, as seen in the Ne IX emission lines in the schematic on the left. The density, absorbing column, shock velocity and turbulence of the gas can then be measured using resonance, intercombination and forbidden lines of He-like ions. At right, we show a comparison of the simulated data from XGS-P for Capella, as compared with archival data from the Chandra/HETG.

The stellar magnetic field and high-energy radiation from young stars ionize the protoplanetary disk and drive accretion via a magnetorotational instability. They also drive gas motions that catalyze planet formation and migration [14]. During the first $\sim 10$ Myr of accretion, the accreting gas absorbs some of the X-ray emission. High-sensitivity X-ray spectra can uniquely determine the intrinsic flux of this impinging radiation by resolving the emission and absorption components of both the shocked and coronal gas. Further, by determining the X-ray flux from
accreting stars onto their protoplanetary disks, the XGS-P would quantify how rapidly the high-energy radiation from young stars disperses their gas disks [15], ending the phase of major planet formation.

2.4 The Importance of Gratings in Context

With the expected launch of XRISM in 2022, we are finally poised to achieve ~5 eV spectral resolution in the ~0.2-15 keV X-ray bandpass with the Resolve microcalorimeter instrument. If the mission follows a timeline similar to Suzaku, we can hope to reap the scientific benefits of this revolutionary detector for ~10 years, providing high-resolution X-ray spectroscopic coverage with ~400 cm² of effective area until the launch of Athena in ~2030. The Athena/X-IFU microcalorimeter will improve on the XRISM/Resolve spectral resolution by a factor of ~2 and on its effective area by a factor of ~30. Critically, however, neither mission will include an X-ray grating spectrometer, thereby losing essential sensitivity below ~2 keV (see Fig. 4). All of the science discussed in the preceding sections and prioritized by Astro2010 would therefore remain inaccessible unless the notional Lynx mission concept is prioritized by Astro2020.

The concept for the XGS-P is timely, as this observatory would realize these Astro2010 priorities with simultaneous access to microcalorimeter data. To characterize the missing baryons, quantify the impact that AGN outflows have on their host galaxies and understand the mechanisms that drive the formation and evolution of stellar systems requires a revolution in sensitivity across the X-ray bandpass, which can be met by the next generation of X-ray grating spectrometers.

3 The XGS-P Observatory

Prior to XGS-P, a concept probe study for a Notional X-ray Grating Spectrometer (N-XGS) was completed in 2012 and is included in the NASA X-ray Mission Concepts Study Project Report (http://pcos.gsfc.nasa.gov/studies/x-ray-mission.php). The N-XGS consisted of a Wolter-1, slumped-glass telescope with a reflection grating array and CCD camera. The optical design of XGS-P would be similar to that of N-XGS, but would take advantage of recent developments in X-ray mirror, grating, and detector technologies. The performance requirements for XGS-P (λ/Δλ > 5000, effective area > 1000 cm², at 653 eV, OVIII Lyα) could be realized in the near future through these technologies. X-ray optics are rapidly advancing, and methods such as those using polished Si optics (§3.2) are capable of fabricating and aligning mirrors to reliably produce optics with PSFs < 5” HEW. Furthermore, diffraction grating technologies (§3.3) are currently at TRL 4 with a clear path to TRL 5. Gratings have recently demonstrated the highest resolving powers [16,17] and diffraction efficiencies [18] measured to date. The detectors (§3.4) would be composed of CCDs and electrical subsystems similar to those used on previous X-ray missions. System level tests incorporating these technologies are already planned and will reduce the most critical technical risk for a Probe mission. Even though developments are currently being made in all the key areas for a grating spectroscopy probe, mission specific developments to reach TRL 6 would still require...
development given the different focal length, module size requirements, alignment budgets, etc. that will be specific to the final design of the XGS-P and unique from what is currently being developed.

3.1 XGS-P Layout

The XGS-P payload consists of an X-ray focusing optic, an array of diffraction gratings, and an array of X-ray detectors at the focal plane. A nominal observatory design is shown in Figure 5. The configuration on the left, labeled A, comprises several full shells of concentric optics to create a Flight Mirror Assembly (FMA). Immediately following the FMA in the optical path is the Grating Array (GA), which disperses the spectrum (the light path is shown as the shaded pink volume) onto an array of detectors known as the Focal Plane Camera (FPC). The GA shown here samples a limited azimuthal span of the telescope. This technique, known as subaperturing [19], capitalizes on the asymmetric contribution of each azimuthal segment of the telescope to the point spread function (PSF). By orienting the GA to disperse along the direction in which the PSF is narrow, the spectral line spread function (LSF) becomes narrower, thus increasing spectral resolving power. If the telescope design is azimuthally modular, then full shells of optics are not necessary for a spectroscopy-dedicated mission and only the modules associated with gratings are included in the FMA as shown in configuration B on the right of Figure 5. The instrument suite consists of two or more independent, objective grating spectrometers operating in parallel. The modular optics utilize several telescope sections contributing to the total collecting area. Each sector feeds an array of gratings that disperse the spectrum onto an array of CCDs. The modular design has several key advantages including: 1) maximizing spectral resolving power by only sampling a fraction of the total telescope PSF, 2) allowing for increased effective area through the incorporation of independently optimized spectrometers, 3) compact design with lower total mass and volume, and 4) repetitive, lower-cost manufacturing processes.

Figure 5: The configuration labeled A shows a full azimuth of concentric optics in the Flight Mirror Assembly followed by a Grating Array that disperses light to the focal plane camera. Configuration B only uses the sections of telescope that are directly feeding the grating array thus limiting the size of the observatory while optimizing performance.

3.2 XGS-P Flight Mirror Assembly

The optics requirements for the XGS-P can be met with a mirror technology being developed at NASA’s Goddard Space Flight Center [20]. The technology combines modern deterministic precision polishing techniques with single crystal silicon to make extremely lightweight mirrors (areal density about 1 kg/m²) with a PSF similar to, or better than, Chandra’s 0.5” half-power diameter
(HPD). In particular, the modular approach, illustrated in Figure 6, of this technology enables XGS-P to realize the advantages mentioned above.

![Figure 6. The four steps of building a large X-ray mirror assembly (drawing not to scale). a: fabrication of a large number of mirror segments, each of which measures approximately 100 mm by 100 mm by 0.5 mm. b: the mirror segments are integrated into many mirror modules each of which contains one to several dozen mirror segments. c: the many mirror modules are then integrated into several meta-shells, which in turn are integrated into the final mirror assembly (d).](image)

This mirror technology is undergoing rapid development. As of June 2019, small mirror modules each containing a single pair of mirror segments have been built and X-ray tested repeatedly, achieving images of 1.3” HPD. These results demonstrate the validity of this approach and its basic technical elements, such as mirror segment fabrication, coating, alignment, and bonding. Upcoming technology development will be focused on perfecting a process to build and test mirror modules containing an increasing number of mirror segments, up to the three dozen or so that are required by the Lynx mission [20]. Once the process of building modules is established, work will begin to develop an engineering process to integrate the modules into a FMA. We expect this technology development to continue to enjoy support from NASA’s Strategic Astrophysics Technology program to meet the requirements of XGS-P and other Probe missions, such as AXIS and TAP. We expect this technology will be ready to support the implementation of XGS-P in the mid to late 2020s for a launch around 2030. The Silicon Pore Optics (SPOs) used in ESA’s Athena mission [21] is a backup, albeit with a modest reduction in resolution.

XGS-P requires >1000 cm² of effective area at 653 eV. Assuming a 50% diffraction efficiency for the gratings [18] and an 80% efficiency for the combination of filters and detectors at the focal plane [17], the effective area requirement for the optics must be 2500 cm². This can be achieved using a 7 m focal length optic with radii from 0.8 m to 1.3 m. The telescope would consist of 75 shells with 4,890 individual polished segments. Such an FMA would have 163 kg of mass for the entire structural assembly.

### 3.3 XGS-P Grating Array

The XGS-P Grating Array could incorporate either reflection or transmission gratings to achieve the performance requirements. Both technologies have been vetted at TRL 4 by the NASA PCOS Technology Management Board and are supported by NASA SAT and APRA funding for development toward future missions such as XGS-P and Lynx.

#### 3.3.1 Reflection Gratings

An overview of a reflection grating in the conical mount is shown in Figure 7. The image on the upper-left shows the geometry of conical diffraction, also known as the off-plane mount [22].
The reflected image is contained within 0th order at angle $\alpha$ in the focal plane and serves as the absolute wavelength reference for the spectrograph. Diffracted light is located at angle $\beta$ according to the generalized diffraction equation,$\sin(\alpha) + \sin(\beta) = n\lambda/[d \sin(\gamma)].$ The diagram shows an array of three gratings protruding out of the page with their grooves shown extended down to the focal plane for illustrative purposes. This demonstrates the radial nature that these grooves must have in order to control grating induced aberrations to the line spread function (LSF). This image also shows the blazed profile that is necessary to preferentially increase diffraction efficiency into the spectral range of interest. This allows for high sensitivity at high dispersion, thus enabling high resolving power concurrently with large effective area to meet XGS-P requirements.

Reflection gratings have been fabricated with precision blaze angles to produce excellent diffraction efficiency [18] as seen in Figure 7. The tested grating has a groove density of 6275 grooves/mm with a blaze angle of $\sim30^\circ$. It has been replicated using UV nanoimprint lithography onto a fused silica substrate and coated with 5 nm of Cr and 15 nm of Au for reflectivity. The measured synchrotron data at the upper right of Figure 7 shows total absolute (reflectivity included) efficiencies $>60\%$ over the XGS-P band. These are some of the most efficient X-ray gratings ever produced and enable the effective area requirements for XGS-P.

Figure 7: a) Conical grating geometry in the extreme off-plane mount. b) Diffraction efficiency measurements showing $\sim60\%$ absolute efficiency from reflection gratings in the X-ray band. c) Spectral resolving power results from high dispersion measurements performed at the PANTER X-ray test facility using 30th order Al K$\alpha$ lines.
To test resolving power capability, radial profile reflection gratings have also been fabricated and tested [17]. The custom groove profile was created using an e-beam lithography tool to write each unique groove individually. The grating was tested in the converging beam of a SPO fabricated by cosine measurement systems [21] using the PANTEK X-ray Test Facility [23]. The tested grating diffracted efficiently out to 30th order using an Al anode electron impact source. The data are displayed as a black histogram with error bars in Figure 7. The dashed red lines give the expected profiles from the 0th order image and the natural line widths of the Al Kα1 and Al Kα2 lines. Adding these lines together gives the solid red line and the spectral resolving power limit. Statistical fits to the data (colored lines) are consistent with a telescope-limited system with a resolving power of R~8000, thus demonstrating the ability of radially-ruled reflection gratings to achieve the R>5000 requirement for XGS-P.

3.3.2 Transmission Gratings

Critical-Angle Transmission (CAT) gratings are blazed transmission gratings with high efficiency in the soft X-ray band. They have heritage from the Chandra High Energy Transmission Gratings Spectrometer (HETGS), but provide ~10X greater diffraction efficiency and blaze into high diffraction orders with demonstrated resolving power > 10,000 [16]. As true transmission gratings they have relaxed alignment and flatness tolerances. They become highly transparent at higher energies (> ~2 keV), which can provide useful data to an imaging camera. CAT gratings can also be conformally coated with thin metal films to extend their bandpass/increase their critical angle [24].

Figure 8: a: Schematic cross section through a CAT grating of period p. The mth diffraction order occurs at an angle $\beta_m$ where the path length difference between AA' and BB' is $m\lambda$. Shown is the case where $\beta_m$ coincides with the direction of specular reflection from the grating bar sidewalls ($|\beta_m| = |\theta|$), i.e., blazing in the mth order. b: Scanning electron micrograph of 200 nm-period deep etch to a depth of 6 µm. c: Grating petal holding four 32x32 mm2 co-aligned CAT grating facets. d: Spectrum of Al–Kα doublet in 18th order from a single Pt-coated CAT grating, measured at the NASA MSFC Stray Light Test Facility (SLTF), demonstrating R > 10,000.

Fabricated CAT gratings consist of freestanding, 200 nm-period, high aspect-ratio grating bars with Level 1 (L1) cross-supports simultaneously etched from the 4-6 µm thick Si device layer of a silicon-on-insulator (SOI) wafer. Blazing is achieved via reflection off the nm-smooth grating bar sidewalls at graze angles below the critical angle for total external reflection (typically in the range of ~1-3° for soft X-rays reflecting off Si). A coarse hexagonal (L2) support mesh is etched from the ~0.5 mm-thick SOI handle layer and serves as structural support for large (up to 32 x 32 mm2 demonstrated size) grating membranes [25]. CAT grating membranes have been bonded to metal flexure frames (comprising a grating facet), subjected to environmental testing (vibration, thermal...
vacuum), and maintained their performance (diffraction efficiency, resolving power) [26]. Measured performance is in good agreement with theoretical predictions, and average absolute diffraction efficiencies of > 31% (including L1 and L2 blockage) have been demonstrated for 4 µm deep gratings [27]. Extending grating depth to ~ 5.5 µm is predicted to lead to efficiencies > 55% (blockage excluded). Etching to 6 µm depth has been demonstrated recently.

During the Arcus NASA Explorer Mission Concept Phase A effort multiple large-area CAT gratings facets were produced. Four facets were aligned to each other in air using a laser-based technique. After alignment they were tested in a spectrometer setup at the PANTER X-ray facility under simultaneous illumination with a pair of co-aligned silicon pore optic units (2.1” FWHM line-spread function) and provided R ~ 3500 [27]. Detailed optical designs and ray-trace models have been developed for both Arcus and Lynx and used to develop error budgets for resolving power and effective area [28,29]. These could be extended to include XGS-P. Near-term development milestones include the fabrication of deeper gratings (~ 5.75 µm) and the optimization of L1 and L2 support structures, all leading to higher effective area.

3.4 XGS-P Focal Plane Camera

The FPC will consist of arrays of photon counting CCDs similar to those flying on Chandra and Suzaku. They will be back-illuminated, grade 0 devices with energy sensitivity of ~100 eV which is adequate to separate overlapping orders from the gratings. Subarcsecond resolution for a 7 m telescope can be obtained with 24 µm pixels with a goal of 16 µm for better sampling. Optical light suppression will be implemented via direct deposition of a blocking filter such as Al onto the CCD surface. Additional contamination control can be implemented using a warm polyimide filter upstream in the optical path. We envision a design with two independent cameras that image two sets of optics and gratings as shown in Figure 5 B. These cameras will be very similar to the N-XGS system which also includes contamination doors and a focusing mechanism to optimize FPC position relative to the optics assembly following launch. The thermal support system for the CCDs consist of a thermal link to dedicated radiators to passively cool the devices combined with heaters and a temperature control system to maintain a stable operating temperature of -90° C. The electrical support systems for the FPC will include detector electronics to provide signal processing and analog to digital conversion. A frame rate of 10 Hz ensures negligible pileup. An event recognition processor will identify photons and digitally process the events to be included in the telemetered data stream. Another unit will be responsible for interfacing the detector electronics to the spacecraft systems.

4 The XGS-P Mission

A full mission design with costing has not been performed for the XGS-P. A proposal was not submitted to the 2016 NASA Astrophysics Probe Mission Concept Study (solicitation NNH16ZDA001N) because the XGS-P was non-compliant due to the previous N-XGS Probe study. The N-XGS went through a full GSFC Mission Design Lab (MDL) session including spacecraft design, mission design, and PRICE-H costing. This white paper serves to ensure that such a probe is considered in the portfolio of Probe-class missions submitted to the Astro 2020 Decadal.

The mission details and cost estimates provided here are based on the MDL outputs for the N-XGS. That concept utilized slumped glass optics for the FMA, as opposed to the polished-Si optics of XGS-P, reflection gratings for the GA, and CCDs for the FPC. The advancements made in the mirror and grating technologies since the time of the N-XGS study require that another MDL
session take place for accurate mission design and costing of the XGS-P; however, we present the N-XGS results here as a baseline estimate for XGS-P until such a study is performed, given the similarity of the payloads.

4.1 Mission Overview
The 7 m focal length of the XGS-P will fit into a Falcon 9 fairing. A 7 m version of the N-XGS was studied as part of the NASA X-ray Mission Concepts Study and is shown within a Falcon 9 fairing in Figure 9. XGS-P would be launched to a Sun-Earth L2 orbit with a three year prime mission and a five year goal. For N-XGS, this orbit over a three year period provided 70 Ms of observation time on science targets. The N-XGS also baselined daily communication with the spacecraft using the NASA Deep Space Network to provide command and telemetry.

4.2 Cost and Basis of Estimate
Costing for the XGS-P has not been performed, but can be estimated from the costing exercise performed for the N-XGS. The cost per WBS element is given in Table 1. The costs were estimated using PRICE-H for total mission lifetime costs. The instrument teams worked with the MDL to produce several outputs including: a baseline design from mission requirements, master equipment lists, interface diagrams, technical readiness assessments, and risk/complexity matrices. The three year total reliability requirement was >85% probability of success. Costs for WBS 1-3 were derived as a percentage of the hardware costs. WBS 1, 2, 3, 5, 6, 7, and 9 all include 30% reserve while WBS 4.1 includes 10% with no reserves in WBS 4.2, 8, and 11.

![Figure 9: The 7 m N-XGS design with a Falcon 9 fairing.](image)

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