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Concepts for High-Performance Soft X-ray Grating Spectroscopy in a Moderate-Scale Mission

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ABSTRACT

We discuss concepts for high-throughput (effective area 250-1400 cm^2), high-resolution (spectral resolving power $R > 3500$) soft X-ray grating spectroscopy in missions of moderate (probe-class or smaller) scale. Such missions can achieve high-priority scientific objectives identified by the Astro2010 Decadal Survey attainable in no other way, and would provide an essential complement to any future large-area X-ray observatory equipped with non-dispersive spectrometers. We enumerate key science drivers and discuss consequences of various alternative design choices for scientific capability and overall mission size.

Keywords: X-ray spectroscopy, gratings, high-energy astrophysics, space astronomy

1. INTRODUCTION

"New Worlds, New Horizons"[1] (NWNH), the report of the US National Research Council's 2010 Decadal Survey in Astronomy and Astrophysics, recommended development of the International X-ray Observatory[2] (IXO) as a high priority for NASA. IXO's scientific appeal stemmed from its very large collecting area and the new capabilities of its science instruments. The core IXO instrument complement included a X-ray micro-calorimeter[3], an advanced wide-field imager[4], and an X-ray Grating Spectrometer[5,6] (XGS). While for various programmatic reasons the international partnership to develop IXO has been dissolved, NASA continues to seek ways to address the scientific questions toward which IXO was aimed[7].

A compelling portion of IXO science was made possible by its XGS instrument. With an effective area exceeding 1000 cm^2 and a spectral resolving power $R \equiv \Delta\lambda/\lambda > 3000$, the IXO XGS was designed to address a broad range of fundamental scientific questions, including "How does cosmic feedback connect the growth of super-massive black holes with that of large-scale structure?"; How does large-scale structure evolve?"; "What happens close to a black hole?"; and "How does matter behave at very high density?" The IXO XGS featured more than an order-of-magnitude increase in effective area over current X-ray spectrometers, and unprecedented spectral resolution.

Here we describe concepts for addressing these questions with missions much smaller and cheaper than IXO. This work was stimulated by recent studies conducted under the auspices of NASA's Physics of the Cosmos (PCOS) program, and focuses on missions dedicated to soft X-ray (0.2- 1.0 keV; ~10 – 60 Å) grating spectroscopy. Specifically, we consider three missions, of three different sizes, each dedicated to grating spectroscopy, that employ similar instrument architectures. The smallest of these, a Warm-Hot Intergalactic Medium Explorer (WHIMex), is an Explorer-class satellite intended for low-earth orbit. The somewhat larger Notional X-ray Grating Spectrometer (N-XGS), and the

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larger-still Astrophysics Experiment for Grating and Imaging Spectroscopy (AEGIS) are probe-class missions designed for operation at L2. The instrumental technology required for these missions is sufficiently advanced that it is envisioned that any of them could begin development by or before the middle of the current decade.

The plan of the paper is as follows. In Section 2 we summarize the advances in scientific capability offered by these next-generation missions, and discuss the scientific motivation for them. In section 3 we review the general instrumental architecture common to all of the instruments we consider, and note alternative approaches for implementing them. In section 4 we describe mission-level implementation details. We conclude with a summary of our findings.

2. SCIENTIFIC CAPABILITIES AND MOTIVATION

High-resolution spectroscopy has provided much of our astrophysical knowledge. The instruments we discuss here will make this technique as powerful in the X-ray band as it has become in other wavebands. Atomic physics makes almost all of the ionization states of all of the abundant elements accessible in the 10 – 60 Å passband, so high-resolution soft X-ray spectroscopy can provide a comprehensive picture often unavailable at other wavelengths.

Grating spectrometers on the Chandra[8] and XMM-Newton[9] observatories have begun to exploit this technique over the past decade, but the missions we consider here are remarkably more capable. Factors of 3-50 more effective area, and three- to ten-fold improvements in spectral resolving power, are envisioned (see Figure 1). The instrument concepts that enable these advances are summarized in Section 3 below. In the remainder of this section we enumerate some of the many scientific questions which have motivated these developments. More complete discussions of the scientific potential of these missions are available elsewhere[†].

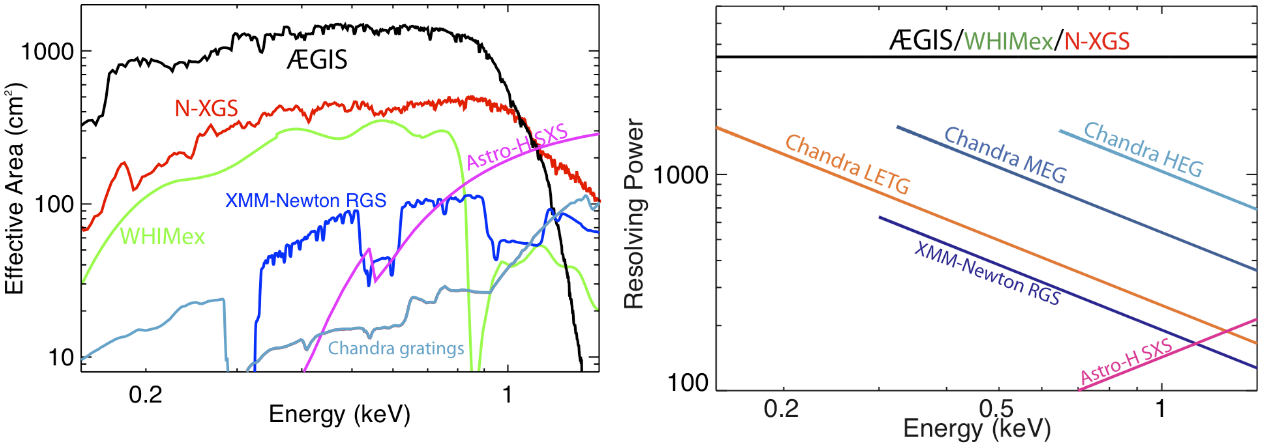

Figure 1: Effective area (left) and spectral resolving power (right) of next-generation grating spectrometers WHIMex, N-XGS and AEGIS far exceed capabilities of instruments operating or in development (XMM-Newton RGS, Chandra HETG and LETG, and Astro-H SXS) over the 0.2-1 keV band.

2.1 How does large-scale structure evolve? Understanding the warm-hot intergalactic medium (WHIM)

More than 90% of the baryons in the local Universe are believed to exist in an extremely tenuous, filamentary structure often called the cosmic web.[10] Half of the cosmic web has been detected by means of far ultra-violet absorption lines of hydrogen (Lyα) and ionized oxygen (OVI)[11, 12], but the vigorous searches have so far failed to detect the remainder. Simulations of the growth of cosmic structure suggest that the as-yet-undetected baryons have been shock-heated to temperatures of 10^{6-7} K in filamentary structures, and possibly enriched by galactic superwinds. This Warm-Hot Intergalactic Medium (WHIM) can be detected and characterized by sensitive X-ray spectroscopy of bright background sources (active galactic nuclei, or AGN) as is illustrated in Figure 2. Detection of lines from ionized carbon, nitrogen, oxygen and neon will yield the distribution of WHIM mass as a function of temperature.

[†] See http://pcos.gsfc.nasa.gov/studies/xray/x-ray-mission-rfis.php

To date, searches with current instruments for soft X-ray absorption lines from the WHIM have been tantalizing but inconclusive[13,14]. The line-detection sensitivity of a spectrometer is proportional to quantity $(A_{eff} \times R)^{1/2}$, where A_{eff} is its effective area and $R \equiv \lambda / \Delta\lambda$ is its resolving power. With substantial increases in both quantities (see Figure 1 above), next generation grating spectrometers will provide factors of ~5 - 10 better sensitivity, as shown in Figure 3. With typical exposure times of ½ to 1 Msec per backlighting AGN, this capability is expected to yield significant (>5σ) detections of several dozens to hundreds of WHIM systems along ~25 -100 different sight lines, depending on the specific mission's effective area.

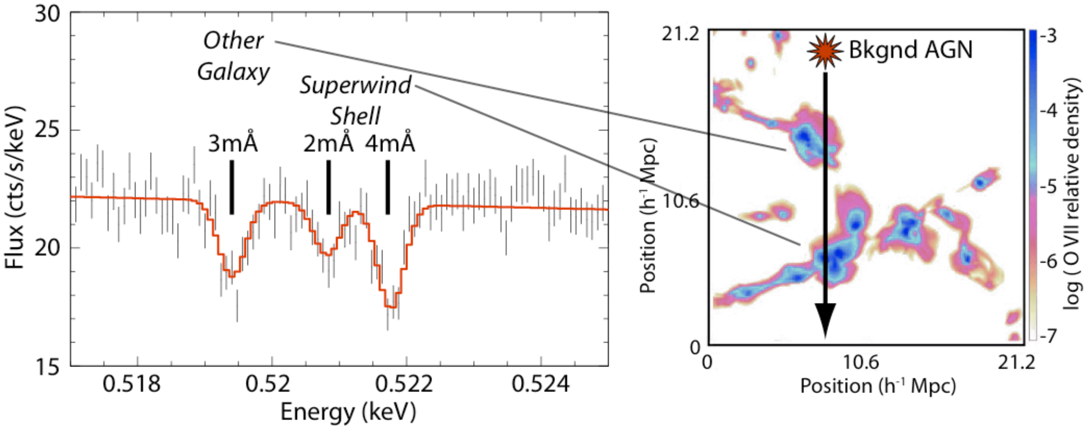

Figure 2: The WHIM can be probed with sensitive high-resolution spectroscopy of background active galactic nuclei (AGN). The observing geometry is illustrated at right; the simulated spectrum, for a 1 Ms exposure to an AGN with flux of 1.5 x 10^{-11} erg s^{-1} cm^{-2} with the N-XGS instrument, is shown at left.

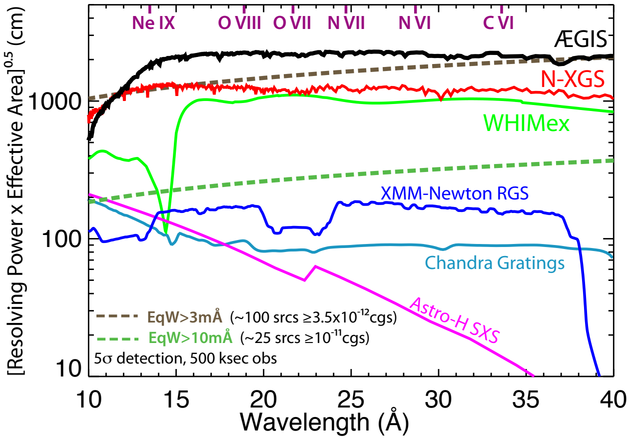

Figure 3: Line detection sensitivity, proportional to $(A_{eff} \text{ x } R)^{1/2}$, is much higher for next generation spectrometers WHIMex, N-XGS and AEGIS than for any existing instrument.

2.2 Supermassive black holes and cosmic feedback

Two key questions identified by NWNH are *"How do black holes grow, radiate and influence their surroundings?"* and *"What are the flows of matter and energy in the circumgalactic medium?"* Both questions address the role of feedback processes in cosmic evolution. Supermassive black holes (SMBH) are known to produce ionized, outflowing winds, and Chandra and XMM grating spectrometers are used to measure the ionization parameters, column densities and velocities of these flows.[15] The key parameters of mass and energy outflow rates, which determine the importance of these winds in shaping the galaxies, cannot be deduced from these data, however, because the density of the wind, and its distance from the source which ionizes it, are poorly constrained. A promising technique for determining wind density is to monitor the timescale on which the ionization state of the wind varies in response to fluctuations in the ionizing source. This method has been used with current instruments to constrain wind density in very bright sources[16,17], but the much larger effective area of next-generation spectrometers is needed to probe a representative sample of objects. These measurements require collection of an adequate number of photons within the timescale on which the sources vary, so they are best accomplished with the mission implementations with the largest collecting area.

A second potential technique for measuring densities at very low levels is to determine ratios of metastable lines such as those of Si X and Si XII (~50.7 Å eV and 36.5 Å , or 245 and 340 eV, respectively) to the corresponding ground states.[18] Current spectrometers have insufficient collecting area at these long wavelengths to exploit this method, but next generation instruments will be able to do so (see Figure 1).

2.3 Matter at very high density

Neutron stars are macroscopic objects of nuclear density, and little is known about the equation of state, and hence the internal structure of these objects. Different equations of state yield different relationships between a neutron star's mass and its radius, and for this reason NWNH highlighted the importance of measuring these two quantities. In principle, high-resolution X-ray spectroscopy of photospheric absorption lines can constrain both mass and radius: the gravitational redshift reveals the ratio M/R, while a Stark-broadened line's width is sensitive to the surface gravity[19] . In practice a key requirement for this measurement is that rotational broadening resulting from the star's spin must be sufficiently small; otherwise the line will be smeared out and rendered undetectable. At least one object with sufficiently slow rotation, the transient IGR J17480-2446, with spin frequency of 11 Hz, has been detected[20], suggesting that a population of slowly rotating neutrons stars does exist.

To date, neutron star photospheric absorption lines have not been reliably detected. Model neutron star atmospheres suggest that the Balmer and Paschen series lines of Fe XXV and FeXXVI (in the 7-13Å and 16-36Å bands) could be expected to have equivalent widths of order ~10mÅ[21]. For such lines to be detected during a typical integrated burst fluence (the produce of burst flux x total burst exposure time) of ~2 x 10^{-5} erg cm^{-2}, a figure of merit $(A_{eff} \times R)^{1/2} \geq 500$-1000 is required at these wavelengths. This is far beyond the capability of existing instruments, but well within the reach for the larger next-generation missions we discuss here (see Figure 3 above).

2.4 Additional Science

High-throughput, high-resolution X-ray spectroscopy will enable scientific advances in many other areas of astrophysics. We list a sampling of these here. The Galaxy's interstellar medium (ISM) will produce absorption features that will allow one to determine the quantity and composition of gas and dust on an element-by-element, and even ion-by-ion basis. This information will improve understanding of a range of astrophysical processes, from nucleosynthesis to planet formation. The structure of the ISM can be mapped in lines of carbon, nitrogen oxygen and neon over lines of sight to hundreds to thousands of Galactic sources (depending on mission effective area), providing a huge advance over the few objects accessible to current instruments. The ISM in as many as ~150 nearby galaxies may be probed as well. The kinematics of material in stellar coronae can be mapped with high precision, leading to better knowledge of coronal magnetic fields, energetics, and ionizing radiation output. In turn, understanding the interplay between coronal flows, ionizing radiation and circumstellar disks improves knowledge of planet formation. The complex physics of accretion on and outflows from neutron stars and stellar-mass black holes can be studied. The larger effective area missions will be most powerful in unraveling these time-varying processes. The two-thirds of the Milky Way's baryons that are so far unaccounted for can be sought in the Galactic Halo and the Local Group and mapped using the same techniques applied to the study of the WHIM. For the larger missions, the search can cover hundreds of sightlines. Diffuse emission from external galaxies can be studied at resolving powers of $R > 300$, providing new information on abundances of carbon and nitrogen and illuminating the origin of metals in these systems.

3. INSTRUMENT CONCEPT

The basic concept for the optical spectrometer itself has been described extensively elsewhere[5,6] and is illustrated in Figure 4. The major components are a Flight Mirror Assembly (FMA), a Grating Array Structure (GAS), and a Focal Plane Assembly (FPA). The FMA contains a Wolter Type-I optic containing segmented, slumped-glass grazing incidence mirrors. Depending on the implementation, the focal length ranges from 4 to 7 m. Outer graze angles for the FMA are relatively large to maximize collecting area in the 0.2 – 1.0 keV band. The blazed, objective gratings are mounted in the GAS immediately behind the FMA, and the dispersed spectra are recorded in the focal plane by the CCD detectors in the FPA. The gratings and detectors are arranged in a Rowland configuration.

As shown in Figure 4, the optical concept entails multiple spectrometers operating in parallel, with each using a fraction of the total mirror collecting area. This scheme has two major advantages. Foremost of these is the improved spectral resolving power resulting from the shape of the image produced by a mirror sub-aperture. Each sub-aperture produces an astigmatic image which can be a factor of several narrower than the half-power diameter of a full-aperture mirror. This effect can be exploited by providing separate spectrometers, each dispersing along the narrow direction of the mirror image (i.e., normal to the plane of incidence of the mirror sub-aperture) for each pair of mirror sub-apertures.

A second important virtue of this design is that it is modular, and can therefore be scaled to fit within a range of different mission cost constraints. WHIMex and N-XGS, for example, each feature 2 spectrometers and require a total of only 1/6 and 1/3, respectively, of a full circular mirror aperture. AEGIS has 6 spectrometers, each fed by 2 30° mirror sectors, and thus uses a full circular mirror aperture. Details of these three configurations are provided in Table 1. The flight mirror assembly uses a segmented mirror architecture originally developed for IXO, and recently deployed on the NuSTAR mission[22,23]. This design is well-suited to the requirement for sub-aperturing. Individual mirror segments are fabricated by slumping thin glass sheets on forming mandrels and coated (with gold or iridium) to enhance X-ray reflectance. Mirror segments are aligned and bonded into modules, and modules are finally aligned and integrated into sectors.

Two different types of grating technology are under development for these missions. Each has been described in detail elsewhere[5,6], and so will only be summarized here. *Off-plane gratings* (OPG) are reflection gratings produced from holographic lithography onto a master substrate which is subsequently replicated onto flight elements to produce the requisite number of gratings. Their efficient packing geometry and blazed profile allow for high throughput while the high density, radial groove profile provides high spectral resolving power. This technology has heritage from the XMM-Newton RGS and suborbital rocket payloads. The effective area and resolving power requirements are typically met using orders 2 through 6. *Critical Angle Transmission gratings* (CAT) are produced from silicon wafers using nanofabrication techniques. They are light-weight, and combine the high spectral dispersion of blazed reflection gratings with the relatively relaxed alignment tolerances of transmission gratings. This technology is a direct descendant of the transmission gratings now flying on Chandra. The CAT spectrometers use a relatively broad range of diffraction orders (nominally 2nd through 12th), and, typically, two different grating periods are used to minimize the variation in effective area with wavelength.

The FPA provides a linear array of X-ray photon-counting CCDs, together with associated electronics, for each spectrometer. The length of the readout and the required pixel size depend on both grating technology and mirror focal length chosen for each mission implementation, as discussed in Section 4. For some CAT grating implementations, a separate CCD, placed at the FMA imaging focus, is required to record the undiffracted (0th order) image. The required CCD pixel sizes (15μm and 24μm) have been demonstrated in flight by HETE-II[24] Chandra[25] and Suzaku[26]. The detectors are back-illuminated for maximum effective area, and must provide sufficient spectral resolving power to separate overlapping orders diffracted by the gratings. The required performance has been demonstrated by the detectors now flying on Suzaku[26]. Detectors must be cooled, nominally to -90°C. The optimum cooling strategy will depend on the mission orbit. The time-resolution and count-rate capability of the instrument is determined by the CCD readout rate, which is specified to be 15 fr s^{-1}.

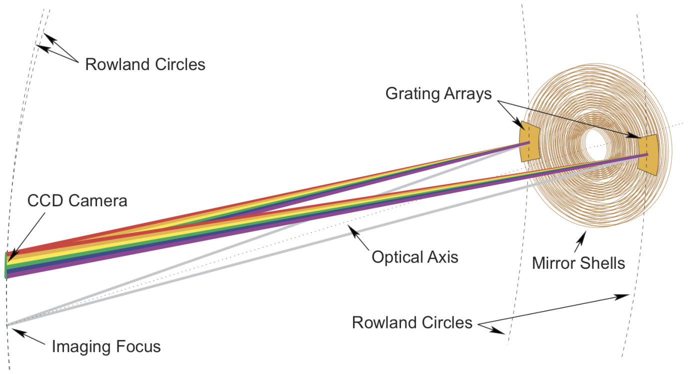

Figure 4: Optical layout of the spectrograph exploits sub-aperturing to maximize spectral resolution. This design is also modular and therefore scalable. In this illustration, one spectrograph is fed by 2 30° mirror sectors. Multiple spectrographs can be included in the instrument to achieve the required effective area.

4. MISSION CONCEPTS

The modular instrument architecture described in Section 3 can be deployed in missions of a variety of scales. Here we summarize mission concepts for WHIMex, N-XGS and AEGIS. Instrument configurations for each mission are described in Table 1. Some significant mission-level parameters are listed for each in Table 2. We briefly discuss each mission in turn.

4.1 Warm-Hot Intergalactic Medium Explorer (WHIMex)

WHIMex was proposed to NASA in 2011 as an Explorer-class mission aimed primarily at investigations of the WHIM and AGN feedback. It has been described in detail elsewhere.[27] WHIMex is the smallest of the mission concepts discussed here, with effective area exceeding 250 cm^2 throughout the 0.2 – 0.8 keV band, with a peak effective area of about 360 cm^2 near 0.5 keV. It is designed for a low-earth orbit (LEO), and could be launched on an Athena 3120.

For maximum spectral resolving power with optics of modest angular resolution (15” HPD), WHIMex baselines a relatively long focal length (F=7m). Off-plane gratings are employed. To accommodate the payload within the volume available in the Athena 3120 shroud, a deployable optical bench is specified. Two parallel spectrometers share a single, 420-mm long, actively cooled CCD readout strip.

4.2 Notional X-ray Grating Spectrometer (N-XGS)

N-XGS is one of several notional missions defined by the X-ray Community Science Team (CST). The CST was commissioned by NASA’s Physics of the Cosmos program office to consider missions at a range of scales that could accomplish high-priority science associated in NWNH with the International X-ray Observatory. All such notional missions were specified to be high-reliability (NASA Class B) observatories rather than single-focus missions. These missions were formulated on the assumption that all required technology would be available (i.e., at technology readiness level 6) in the middle of the current decade.

The baseline optics adopted for N-XGS are assumed to provide angular resolution of 10” HPD, and thus resolving power requirements can be met in a relatively compact (F=4m) design. Point designs for both OPG and CAT gratings have been developed with these optics. Resource requirements for the OPG version are summarized in Table 2, as these are expected to envelope those required for the mission.

N-XGS has two spectrometers operating in parallel. Each is fed by annular mirror sectors occupying 60° of a full circle, and each requires a 300mm-long, passively-cooled readout strip. N-XGS has an effective area somewhat larger than that of WHIMex, and was configured to operate in an L2 orbit, which is expected to provide greater observing efficiency than is at available in LEO. As a larger and more expensive observatory than WHIMex, N-XGS would be capable of addressing a broader range of scientific topics.

4.3 Astrophysics Experiment for Grating Imaging and Spectroscopy (AEGIS)

AEGIS, (an Astrophysics Experiment for Grating Imaging and Spectroscopy) was described in a white paper submitted to NASA in response to its 2011 Request for Information on concepts for future X-ray astronomy missions[‡]. The largest of the three missions discussed here, AEGIS adopts a filled circular mirror with 10” HPD and 4.4m focal length. CAT gratings, which provide the minimum mass-to-area ratio, are adopted for this large-area design. Each of six parallel spectrographs is fed by a pair of diametrically opposed, 30° mirror sectors. Each spectrograph is served by a 100mm-long, passively cooled readout array. This configuration provides effective area exceeding 1400 cm^2 at 653 eV. Detailed ray-tracing methods and results for AEGIS are presented in a companion paper in these proceedings[28]. AEGIS, like N-XGS, it is configured for deployment at L2 as an observatory-class mission. AEGIS’s large effective area, coupled with the high observing efficiency of the L2 orbit, provides the greatest scientific capability of the three missions discussed here.

[‡] See http://pcos.gsfc.nasa.gov/studies/xray/x-ray-mission-rfis.php

Table 1: Instrument Parameters

Parameter	WHIMex	N-XGS	AEGIS	Remarks
Total effective area, cm^2	320	500	1440	OVII Lyα, 653 eV
Spectral resolving power	>3500	>3500	>3500	
Number of spectrometers	2	2	6	
Mirror focal length, m	7.0	4.0	4.4	WHIMex employs a deployable bench
Grating type*	OPG	OPG or CAT	CAT	
Grating period (nm)	180	167 (OPG) 200 & 230 (CAT)	200 & 230	N-XGS can be configured for OPG or CAT
Readout characteristics: total length (mm) pixel size (μm) readout rate (fr s^{-1})	 420 15 ~0.2	 300 24 15	 100 24 15	Back-illuminated CCD detectors

*OPG: Off-plane grating; CAT: Critical Angle Transmission Grating

Table 2: Mission parameters

Parameter	WHIMex	N-XGS	AEGIS	Remarks
Payload mass (kg), CBE*	175	240	325	Includes optics, excludes structure, WHIMex DOB*
Launch mass (kg)	660	830	1090	Incl. 30% reserve
Orbit	LEO (540 km)	L2	L2	
Launch vehicle	Taurus 3120	Falcon-9	Falcon-9	
Mission Class	Explorer/Class D	Probe/Class B	Probe/Class B	
Mission Lifetime (years)	3-5	3-5	3-5	

*CBE: Current best estimate; DOB: Deployable optical bench

5. DISCUSSION

The two critical instrument performance characteristics for these missions are effective area and spectral resolving power. All of the missions we discuss provide substantial increases (factors of 3-10) in effective area relative to current instruments (see Figure 1). The effective areas of WHIMex, N-XGS and AEGIS span a large range (slightly more than a factor of 3). A secondary, but important factor distinguishing WHIMex from N-XGS and AEIGS is the greater observing time available to the latter two at L2.

Remarkably, all three missions provide similar resolving power (R >3500). The improvement over current instruments (a factor of at least 3) is crucial: next generation grating spectrometers will be the first to resolve the thermal line-widths at E < 1 keV in hot (~10^7 K) plasmas.

A comparison of these missions with IXO is revealing. Table 3 lists the product of available exposure time and band-averaged effective area ($\bar{A}_{eff} \times T_{XGS}$) for each, along with that for IXO. For the latter we assumed, in accordance with the nominal IXO observing plan, that about 15% of the 5-year IXOmission at L2 would be devoted to grating (XGS) observations. The total number of photons collected is proportional to the $\bar{A}_{eff} \times T_{XGS}$ product, and given that all of these spectrometers have comparable spectral resolving power, this figure of merit accurately reflects the scientific power of the instrument when temporal variations of the objects under study are small or uninteresting. Scientific problems in this category include probing the WHIM, searching for the Galaxy's missing baryons, or studying the interstellar medium. Table 3 shows that, for such questions, *all of the missions we consider offer at least as much, and in two cases significantly more high-resolution grating spectroscopy capability than IXO would have provided.*

With larger effective area than WHIMex, N-XGS and AEGIS can address a broader range of such topics, and/or probe them to greater depth (e.g. with a larger number of lines of sight through the WHIM), within their mission lifetimes. Moreover, N-XGS, and even more so AEGIS, have a qualitative advantage in doing science for which source variability is important. Examples include studies AGN winds through ionization variability, probing the accretion physics of binary X-ray sources, studies of the evolution of stellar coronae, and probes of the neutron star equation of state.

Table 3: Integrated Effective-area x exposure-time product for grating spectroscopy with various missions.

Mission	**Observing Efficiency**	**XGS Fraction**	**Band-averaged Effective Area ($\bar{A}_{eff}$, cm^2)**	**Mission XGS Exposure (T_{XGS}, Ms)**	**Area x Exposure ($\bar{A}_{eff} \times T_{XGS}$, 10^9 cm^2 s)**
IXO (XGS)	75%	15%	1000	18	18
WHIMex	60%	100%	300	57	17
N-XGS	75%	100%	450	71	32
AEGIS	75%	100%	1100	71	78

6. SUMMARY

We have described concepts for three missions of modest scale that are dedicated to high-resolution spectroscopy in the 0.2 – 1.0 keV band. We have discussed some of the important scientific questions these missions can address. We have outlined a modular spectrograph architecture that allows effective area to be tailored to satisfy mission size and cost constraints. The missions we describe offer capabilities that are, by important measures, comparable or superior to those of the IXO X-ray Grating Spectrometer at much smaller scale. They are capable of achieving a wide variety of high-priority scientific goals identified by the Astro2010 Decadal Survey in Astronomy and Astrophysics.

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