

Curved Diffractive X-ray Optics for X-ray Astronomy

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ABSTRACT

We report on a concept for curved diffractive X-ray optics (CDXO). CDXO would enable potential new optical designs for X-ray instruments, such as a two element spectrometer, in which the secondary element of an X-ray mirror pair is patterned with an X-ray grating. A two-element spectrometer design eliminates the grating assembly, resulting in decreased instrument mass and reduced power requirements. In addition, a two-element spectrometer may realize cost/schedule savings by eliminating a separate grating alignment effort, and yield increased effective area over three element designs. We present a raytrace concept study of a two-element spectrometer compact enough to fit within a sounding rocket payload. We also review the progress made in electron-beam lithography (EBL) techniques that would enable curved diffractive X-ray optics to be patterned, and outline a procedure by which the accuracy of the EBL patterning process can be measured interferometrically.

Keywords: diffraction gratings, electron beam lithography, freeform optics, X-ray spectroscopy

1. INTRODUCTION

High-throughput, high-resolution X-ray spectroscopy can address many of the key questions posited by the 2010 Decadal Survey and NASA's 2013 Astrophysics Roadmap. The 2013 Astrophysics Roadmap¹ specifically identifies spectroscopic capability as a critical component of a notional X-ray mission, as it enables "detailed studies of plasma states and interactions, motion, substructure, and turbulence." Moreover, the *New Worlds, New Horizons* Decadal Survey of Astronomy and Astrophysics² identifies several critical science questions that can be uniquely addressed by X-ray spectroscopy: 'How do black holes grow and impact their surroundings?'; 'How do stars accrete, and how do hot star winds influence their local environments?'; 'How do baryons cycle in and out of galaxies?'

To address these inquiries, numerous X-ray spectrometer concepts have been formulated over the past decade e.g. *WHIMex*;³ AEGIS;⁴ OGRE;⁵ *Arcus*;^{6,7} *Lynx*.⁸ Each of these proposed missions uses three optical elements in its design: a primary and secondary mirror assembly, plus a grating assembly. For each of these missions, the gratings proposed are either X-ray reflection gratings⁹ or critical angle transmission (CAT) gratings.¹⁰ While CAT gratings and X-ray reflection gratings employ grating assemblies arranged in curved geometries (e.g. a Rowland Torus¹¹) to realize a high-resolution spectrometer design, the gratings themselves are planar, being manufactured from silicon wafers.

In the present work, we explore the design and fabrication implications of curved diffractive X-ray optics (CDXO), in which an X-ray grating is patterned on a curved substrate such as a mirror or lens. CDXO opens new optical design space for X-ray instruments, and would enable X-ray spectrometers with only two elements: a primary mirror assembly and a dispersive secondary assembly. In reducing the number of photon interactions within the instrument, a two-element spectrometer may be able to offer improved throughput over three-element designs. In addition, a two-element spectrometer would have reduced mass due to the elimination of the grating

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assembly, and may be simpler to align, assemble, and thermally control. We report on an initial optical design for a two-element spectrometer, as well as discuss potential methodologies for fabricating and characterizing CDXO prototypes.

2. SCIENCE IMPACT

As an example of the unique scientific return offered by a high-resolution X-ray spectrometer with high effective area, we expand on the Decadal Survey question: ‘How do baryons cycle in and out of galaxies?’ Most ($\sim 95\%$) of the baryons in the Universe exist in gaseous form. At low redshift, the warm-hot intergalactic medium (WHIM) is a significant reservoir of baryonic material. Recent studies^{12,13} have detected WHIM filaments via the Sunyaev-Zeldovich (SZ) effect in stacked galaxy measurements; however, most of the constraints on the WHIM are derived from absorption line studies. UV absorption line studies of the ‘warm’ phase ($\lesssim 10^{5.5}$ K) have placed constraints on its mass content (20 – 40%).^{14,15} The ‘hot’ phase ($\gtrsim 10^6$ K) is thought to contain more of the low- z baryons, accounting for as much as 50% of the total and 90% of metals.^{16,17} Observing these absorption lines is more than an exercise in accounting for this ‘missing’ component of baryonic mass, as conditions driving the formation and evolution of large-scale structure are imprinted on this hot phase of the WHIM. For example, the space density of absorption systems (dN/dz) as a function of equivalent width can be calculated from cosmological simulations and compared to an observational survey of WHIM filaments, thus providing constraints on models of the evolution of large scale structure.¹⁸

At the temperatures of the ‘hot’ phase, astrophysically abundant metals contribute to the X-ray spectrum predominantly through bound-bound lines.²⁰ The resonance line of O VII (574 eV) and the Ly α equivalent in O VIII (654 eV) are promising transitions for the detection of WHIM filaments, and these absorption lines should be detectable in the spectra of bright background AGN^{18,19} (Fig. 1). Recently, X-ray absorption lines from the hot phase of the WHIM have been convincingly observed in the spectrum of H1821+643.²¹ However, the method employed detects the absorption line without resolving individual filaments relying on the *a priori* redshifts of measured UV absorption line systems, and employing stacked *Chandra* LETG spectra along a well-observed (470 ks) sightline to generate a 3.3σ detection. Thus, while this detection lends credence to using X-ray absorption line spectroscopy to characterize the ‘hot’ phase of the WHIM, it also demonstrates the limitations of current instrumentation to perform these absorption line studies. To generate a statistical sample of filaments, *Bregman et al.* (2015)¹⁸ outline an observational strategy with a notional X-ray spectrometer with minimum performance requirements of spectral resolution $R \geq 2000$ and effective area $A_{eff} \geq 300$ cm². These requirements exceed the capabilities of *XMM-Newton* or *Chandra* – this resolution is $4\times$ better and the effective area $10 - 100\times$ larger than offered by these instruments in the relevant wavelength range.

3. TWO ELEMENT SPECTROMETERS

3.1 Effective Area Estimate

In this scientific context, we estimate the effective area of a two-element X-ray spectrometer design featuring CDXO. As a point of comparison, we adopt the effective area of *Arcus*, a Medium-class Explorer concept selected for Phase A study²² for both designs. The proposed *Arcus* design uses SPO²³ and critical-angle transmission (CAT) gratings¹⁰ to achieve an effective

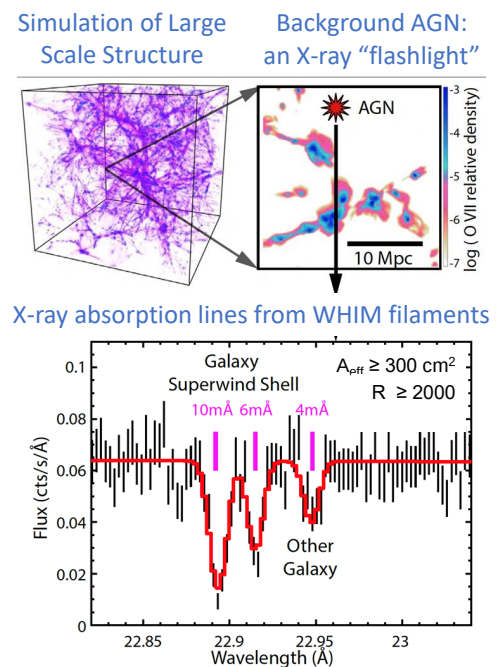


Figure 1: A high-resolution with X-ray spectrometer high effective area can probe the physical properties of the hot phase of the WHIM. These measurements help constrain models of large-scale structure formation and feedback. Figure adapted from Brenneman et al. 2016.¹⁹

area of $> 250 \text{ cm}^2$ and a resolution of $R > 2500$ over the $21.6 - 28 \text{ \AA}$ bandpass, thus meeting the performance requirements outlined for the hot baryon census.

A comparable two-element design for Arcus would employ diffractive SPO XOUs, in which the secondary stack within an SPO is patterned with an X-ray grating. From the *Arcus* effective area, we estimate the performance of this two-element design by (1) dividing the estimated *Arcus* effective area by the semi-empirical diffraction efficiencies for the CAT gratings ($\sim 40\%$ absolute efficiency) and the reflectivity of one SPO interaction ($\sim 90\%$ reflectivity) and (2) multiplying by the measured diffraction efficiency of X-ray reflection gratings made using an EBL technique ($\sim 70\%$),²⁴ making the implicit assumption that the efficiency for diffractive SPO XOUs and existent reflection gratings would be comparable.

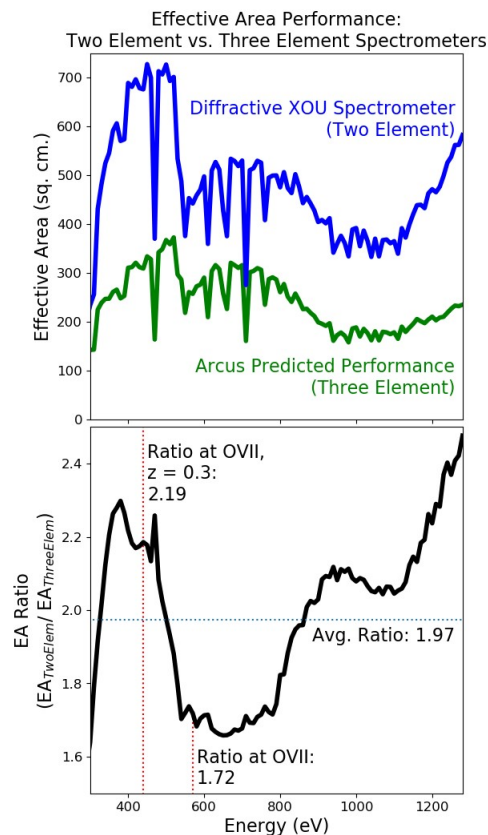


Figure 2: An estimate of the improved effective area that a two-element design could offer the Arcus mission. The dips visible in instrument EA are due to physical gaps in the CCD detector array.

on the CDXO. This raytrace is then wrapped in a numerical optimization routine in order to minimize the RMS diameter of the diffracted line spread function (LSF) at a specified focal plane location.

We select the effective wavelength ($n\lambda$) for optimization as $83.4 \text{ \AA}$. This was chosen to facilitate X-ray testing at 10th order with an Al $K\alpha$ emission line source ($\lambda = 8.34 \text{ \AA}$), and roughly corresponds to observing O VII absorption lines at 4th order. For the spectrometer geometry, we adopt the optical prescription of the OGRE sounding rocket.²⁶ The OGRE X-ray spectrometer baselines using mono-crystalline silicon optics^{27,28} and X-ray reflection gratings to form an X-ray spectrometer with modest resolution and effective area ($R > 2000$, $A_{eff} >$

Fig. 2 shows that a two-element design offers a factor of two improvement averaged across the soft X-ray bandpass. Thus, in the case of *Arcus*, we calculate that a two-element spectrometer design can roughly double the effective area while modestly reducing the instrument mass by eliminating the grating subassembly. Alternatively, the number of optical channels in *Arcus* could be reduced from four to two, thus performing the same science while having $\lesssim 50\%$ the optical assembly mass.

3.2 Initial Optical Design

CDXO form the base optical units of a two-element spectrometer design. To explore the design space and assess the resolution offered by this concept, a raytrace study which optimizes the grating pattern required for the diffracting secondary X-ray mirror and computes the resulting resolution was performed. The grating pattern for a CDXO has to compensate for the curvature in both the axial and azimuthal dimensions of the X-ray mirrors while maintaining constant dispersion. To have enough free parameters in the optimization, both the groove density and the local orientation of the grooves must change over the surface of the optic. In other words, making a CDXO will require (1) patterning on the curved surface of an X-ray mirror, (2) patterning grooves with variable line spacing (VLS) and (3) patterning grooves with a relative angular offset.

For the proof-of-concept raytrace study of two-element spectrometers, we adopt the Wolter-I geometry²⁵ commonly employed for X-ray telescopes. Based on this geometry, we then developed a custom raytrace to simulate a Wolter-I primary and a diffractive Wolter-I secondary as the CDXO. As we are interested in assessing the limiting resolving power performance of a two element design, we assume idealized mirror pairs free of optical error i.e. the point-spread function (PSF) of the Wolter-I mirror is infinitesimally small. The CDXO raytrace takes functions specifying the periodicity and angular orientation of the grooves at a given point

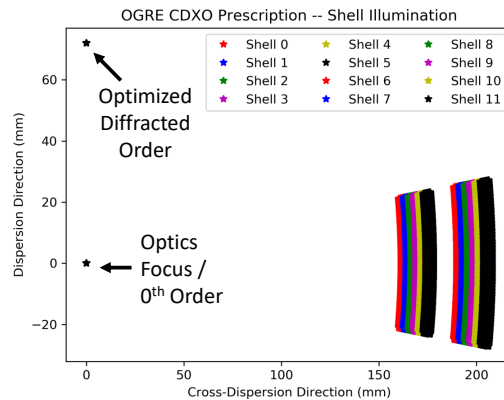


Figure 3: The diffraction geometry for the OGRE two-element spectrometer. The twelve distinct mirror shell pairs are seen on the right. Rays arriving at the focus are shown at (0 mm, 0 mm), while the optimized diffracted LSF is shown at (0 mm, 72 mm). The optimized LSF has a size of a few microns, and hence contributions from each individual shell are indistinguishable at the plotted scale.

35 cm²) in a compact package. The instrument's telescope consists twelve segmented mirror pairs with a focal length $z_0 = 3500$ mm and radii r_0 ranging from 165 - 195 mm.

Given this geometry, we elect to optimize the diffracted LSF at location displaced 72 mm azimuthally relative to the center of the mirror pairs, and optimize for a focal plane normal to the optical axis at the same focal distance ($z = 3500$ mm) of the focus of the optics (0th order). This diffraction geometry is visualized in Fig. 3. We note that, as the grating patterns of the CDXO are numerically optimized based on this focal plane selection, a system featuring CDXO offers additional flexibility in specifying the location of its detectors. In contrast, a three-element spectrometer requires a curved focal plane for high-resolution.¹¹

The LSF resulting from the optimization is shown in Fig. 4, while an example of the computed CDXO grating pattern yielding this solution is shown in Fig. 5. The RMS diameter of the optimized LSF is ~ 3 micron (0.18 arcseconds), which is consistent with the diffraction-limit for a telescope of this prescription. Hence, this design is capable of offering telescope-limited resolving power of $R \gtrsim 15000$. As for the grating pattern itself, the CDXO requires periods ranging from 394 - 409 nm and a total variation in groove orientation of $\sim 0.2^\circ$. Both these variations are of the same order of the values required for conical X-ray reflection gratings, which have period variations of order tens of nanometers and fan angles of $\sim 0.4^\circ$ over similar size formats.

4. CDXO FABRICATION METHODOLOGY

Given the similarity between the required CDXO grating patterns and the patterns written via electron-beam lithography (EBL) for conical X-ray reflection gratings, initial studies of CDXO fabrication center around EBL patterning on curved substrates. EBL offers a flexible patterning method to achieve the required critical dimensions for an X-ray grating ($\sim 100 - 400$ nm). EBL employs a beam of accelerated collimated electrons to deposit energy into a resist layer. Above a certain threshold of deposited energy, the resist can be developed in specific solvents and the recorded pattern exposed. While establishing the correct dose requires a characterization run prior to patterning a substrate, this dose is a function of the EBL column settings and the resist employed, and is largely independent of the pattern to be recorded. In other words, assuming that the correct dose is well-established, there is little to no overhead for changing the pattern to record. EBL is capable of patterning small feature sizes, with isolated features of < 10 nm in extent routinely demonstrated,²⁹ and performing patterning over wafer-sized areas (≥ 100 cm²). Given that it can pattern small feature sizes over large areas and offers flexibility in patterning with little overhead, EBL is well-suited to the challenge of producing X-ray gratings with distinct optical prescriptions as would be required in two-element spectrometer designs.

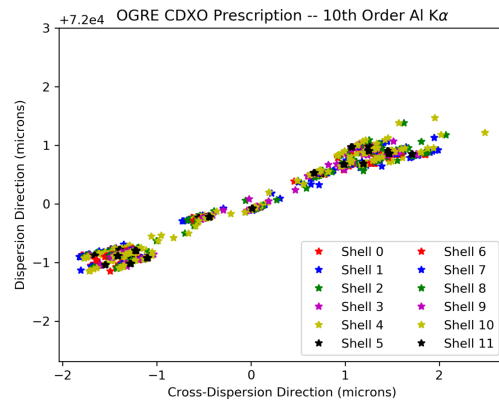


Figure 4: The resulting LSF from the raytrace optimization. This plot is produced by illuminating each shell of the spectrometer with a grid of rays distributed over the radial and azimuthal extent of each shell. The resulting LSF has a RMS diameter of ~ 3 micron, which corresponds to 0.18 arcseconds at this focal length.

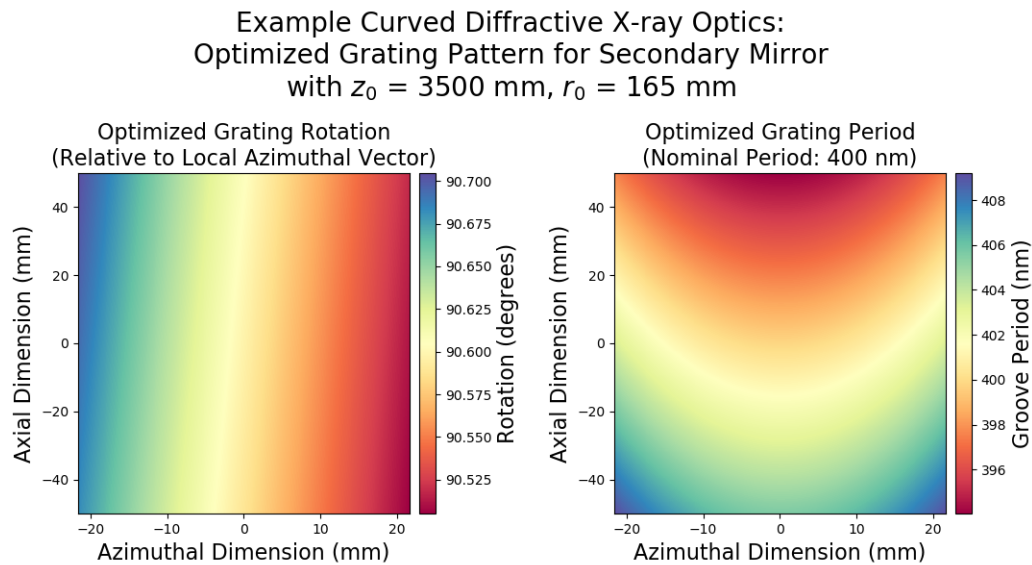


Figure 5: An example of a calculated CDXO grating pattern. This CDXO pattern is taken from the innermost OGRE mirror pair (radius: 165 mm), and is plotted over the azimuthal and axial extent of the mirror.

EBL has been previously employed in the manufacture of X-ray reflection gratings operated in a conical mounting.^{30–32} In this mount, the plane of incidence of the incoming photon contains the groove direction of the grating. Because the focus of an X-ray telescope is converging azimuthally (i.e. in the dispersion direction of the grating), the grating grooves must match this convergence to achieve high-resolution, such that the grating grooves would all intersect at a single fictional hub point. In essence, then, an conical X-ray reflection grating requires a pattern with variable line spacing (VLS), in which both the groove density and the groove direction change as a function of position on the grating. Large-format conical X-ray reflection gratings have been previously patterned with EBL and demonstrate high resolving power during X-ray testing,⁸ implying that EBL is capable of producing the period / groove orientation variations required for CDXO.

In addition to requiring period and groove orientation variations, gratings for two-element spectrometers will also need to be patterned on the curved surfaces of X-ray mirrors. Mirrors proposed for other soft X-ray spectrometers (e.g. *Arcus*, *OGRE*) have a sag of approximately 2 - 3 mm. EBL has previously been employed to manufacture curved gratings with sags and periodicities comparable to those needed for the diffractive X-ray optics required for two element spectrometers. EBL patterning on curved substrates is an established technique in visible and infrared wavelengths.^{33,34} For example, a curved, blazed optical/near-infrared grating was fabricated using EBL for the CRISM instrument on the Mars Reconnaissance Orbiter.³⁵

5. FUTURE WORK

Establishing a method for fabricating curved gratings via EBL is a crucial next step in the maturation of the CDXO concept. Studies to write grating patterns on curved substrates using a Raith EBPG5200 EBL tool, the same tool used to pattern conical X-ray reflection gratings, are ongoing.³⁶ As a starting point, these studies will develop a method of lithographically patterning small areas ($\sim 25 \text{ mm}^2$) on curved lenses. The pattern within these small areas can be ‘spot-checked’ with a Scanning Electron Microscope (SEM).

Following this initial process development, we will optimize the process for large areas and apply it to manufacture large ($\sim 2000 \text{ mm}^2$) optical gratings on curved lenses. Large format optical lenses are commercially available from a number of optics manufacturers, often at costs comparable to silicon wafers. By fabricating specific groove patterns on cylindrical and spherical substrates and interferometrically measuring the diffracted wavefront produced by the grating, the groove placement accuracy of the curved EBL process can be assessed. This technique of interferometrically measuring gratings in back-diffraction has previously been employed to assess the fidelity of gratings written on flat substrates, as the measured planarity of the wavefront can be directly mapped into groove placement or orientation errors.^{37,38}

For a cylindrical substrate, we have calculated a grating pattern which produces a planar wavefront when measured by an interferometer in back-diffraction i.e. when the wavefront from a diffracted order proceeds back along the path of the incident wavefront (Fig. 6(a)). The underlying figure of the cylindrical substrate can be independently accounted for by measuring its figure using a computer generated hologram (CGH) cylindrical null. Due to the axial symmetry in this geometry, the back-diffracting grating pattern does not require the groove orientation to change over the substrate. This makes a cylindrical grating suitable for assessing the groove placement accuracy of patterning at variable heights independently from patterning errors that might be introduced from patterning grooves with different angular orientations.

Patterns for spherical gratings, on the other hand, require both a VLS pattern and grooves that change angular orientation across the substrate to account for the change in curvature, making them similar to CDXO patterns. An example of such a grating pattern and optical test configuration is given in Fig. 6(b). The spherical grating’s figure can be independently characterized and removed using a spherical null. While the grating patterns for these back-diffracting optical gratings on curved substrates have periods larger than those for CDXO, the periods are within a factor of $3\times$ required for CDXO while exhibiting greater groove angular variation ($\sim 10^\circ$) needed. Thus, these cylindrical and spherical gratings made during this phase of the study represent an intermediate technological step, and inform the application of the merged EBL process to CDXO.

In parallel with these EBL patterning studies, we are also working on expanding the proof-of-concept raytrace to quantify the impact of optical system errors, including mirror figure, mounting distortions, and misalignments, and the impact of testing with an X-ray source located at a finite distance. Incorporating these additional

features will be facilitated by transferring the raytrace and optimization to the UI High Performance Computing (HPC) cluster, resulting in more time-efficient computation. Conducting these studies of EBL patterning on curved substrates will provide an early assessment of the viability of the CDXO fabrication, while more detailed raytracing studies can more firmly establish the performance capabilities and potential drawbacks of optical designs featuring CDXO.

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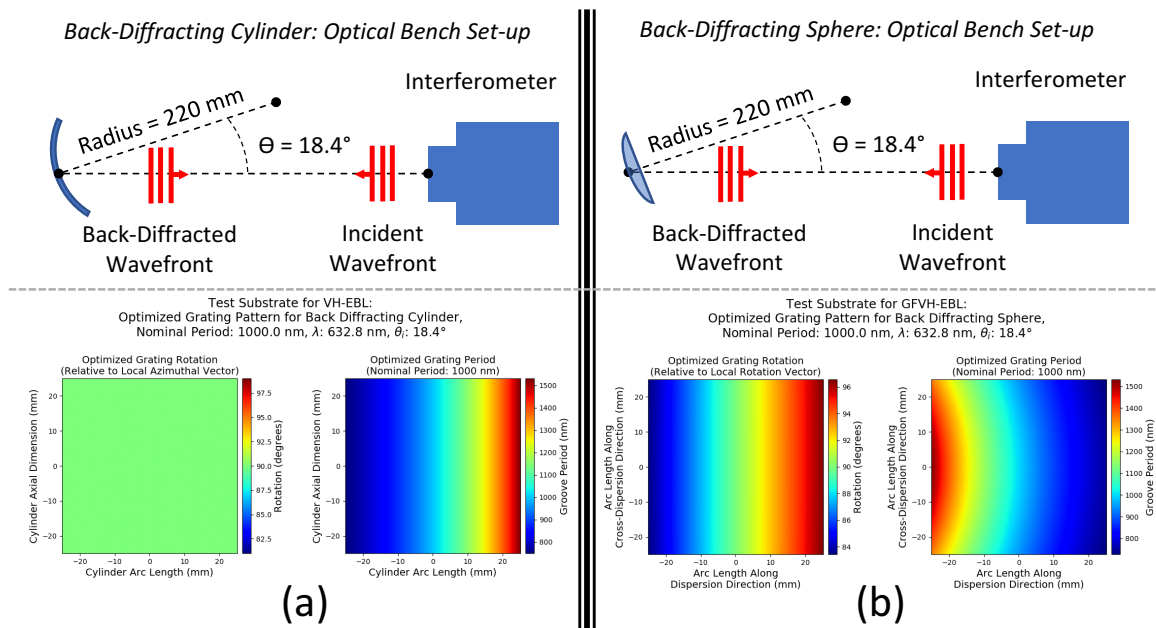


Figure 6: (a) The optical bench set-up (top) and the required grating pattern (bottom) for an example back-diffracting cylinder. Note that the grating grooves do not need to change orientation in this instance, and hence only requires producing a VLS pattern while compensating for the sag of the optic. (b) The optical bench set-up (top) and the required grating pattern (bottom) for an example back-diffracting sphere. This grating shares similarities with CDXO patterning, requiring both the periodicity and orientation of the grating grooves to vary over a curved surface. By fabricating large-format optical gratings using EBL and measuring them interferometrically, the EBL patterning accuracy for CDXO can be quantified without requiring X-ray testing.

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