Performance simulations for the ground-based, expanded-beam X-ray source BEaTriX

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ABSTRACT

The BEaTriX (Beam Expander Testing X-ray) facility, being assembled at INAF-Brera Astronomical Observatory, will represent an important step in the acceptance roadmap of Silicon Pore Optics (SPO) mirror modules, and so ensure the final angular resolution of the ATHENA X-ray telescope. A paraboloidal mirror, manufactured at INAF-Brera, will provide a collimated X-ray beam to a monochromating system and to a beam expansion unit, enabling the full illumination of the mirror modules under test with a broad, highly monochromatic, and parallel X-ray beam. Such a beam will be used to directly diagnose SPO modules in their focusing performances. This requires, indeed, the expanded beam to have a divergence smaller than the expected angular resolution of the modules under test. This condition is subject, in turn, to the optical quality and to the alignment of the optical components. Aiming at establishing the final angular resolution that can be reached and the respective fabrication/positioning tolerances, we have been dealing with a comprehensive set of optical simulations. Modeling based on wave optics and ray-tracing was carried out to predict the collimation performances of the paraboloidal mirror, including the effect of surface errors obtained from metrology. Ray-tracing routines were subsequently employed to simulate the full beamline. This paper reports the simulation results and the methodologies we have adopted.

Keywords: BEaTriX, X-ray test facility, collimating mirror, optical simulations, wave optics, ray-tracing

1. INTRODUCTION

On-ground test and calibration of imaging optics for X-ray telescopes have always posed a problem. First, they require large vacuum systems to accommodate optical systems that have become increasingly large over time. Secondly, the large focal lengths at play not only require a long range in vacuum; the oncoming beam has to be highly collimated (e.g., nearly parallel) to simulate the incidence from a source at virtually infinite distance. Since X-rays are hardly handled by means of refractive systems, this requirement entails locating the source at very large distance - like PANTER at MPE,[1] or the XRCF beamline at MSFC - with a further increase in the vacuum volume and the pumping-down time. Even though these two facilities represent worldwide reference points in the calibration of astronomical X-ray optics, they are hardly adoptable to perform the individual tests of the more than 600 elements that will compose the imaging module of the ATHENA X-ray telescope.[2]

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The ATHENA (Advanced Telescope for High-ENergy Astrophysics) X-ray telescope is the second large mission selected by ESA within the Cosmic Vision Program, with launch scheduled in the early 2030s. It will be the largest X-ray telescope ever built, with a 2.5 m diameter, a 1.4 m^2 effective area at 1 keV, and an angular resolution of 5 arcsec half-energy width (HEW). Such a large focusing system cannot be manufactured with monolithic mirrors; it will be populated with modular elements, termed as MMs (*mirror modules*), based on *silicon pore optics* (SPO), a technology conceived and developed by ESA and the *Cosine* company (Warmond, The Netherlands), where SPO MMs will be manufactured in series.[3] After manufacturing, however, the focusing properties of MMs need to be qualified through a measurement of their *point spread function* (PSF) and *effective area* (EA). Currently, tests of SPO MMs are performed at the XPBF 2.0 beamline of the BESSY II light source.[4] Nevertheless, the beam at BESSY is too small to enable a full illumination of the MM aperture in a single shot, and the characterization is achieved by scanning the optical element and reconstructing the PSF.[5] Full aperture measurements of SPO MMs have been performed at PANTER[6] to validate the qualification process ongoing at BESSY. Despites, a routinely and systematic qualification of the mirror modules coming from the production pipeline, at a foreseen rate of 2-3 MMs/day, demands a dedicated facility with reduced vacuum-venting cycles and able to generate a parallel and wide X-ray beam.

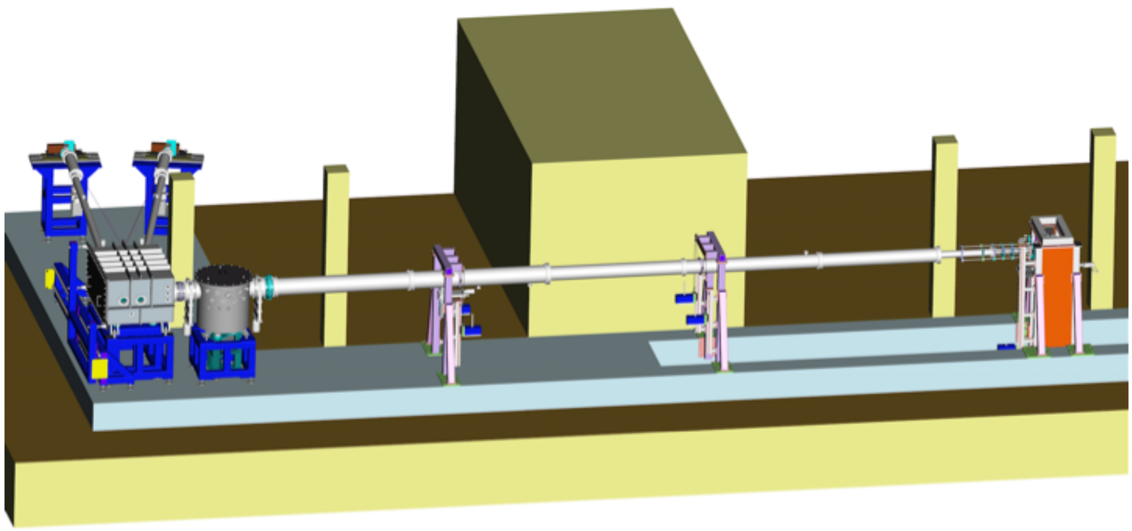

Figure 1: final layout of the BEaTriX facility (Tecnomotive design). The two short arms foreseen for the two X-ray energies (4.51 keV and 1.49 keV) are visible on the left side of the picture. The squared optical chamber houses the optical elements that filter, collimate, and expand the beam to a 17 cm × 6 cm size. The cylindrical chamber will enclose the MM to be tested, whose focus will be inspected right at the end of the long arm (left to right in the picture). All the components are under vacuum (10^{-6} mbar).

These motivations urged us to design and develop the BEaTriX (*Beam Expander Testing X-ray facility*) system[7] with the specific purpose of performing the functional tests of SPO modules prior to their integration into the mirror assembly of ATHENA. Following a number of updates over years,[8][9][10] BEaTriX has been finalized (Figure 1) in its design[11] and, owing to a number of grants (ESA, AHEAD, ASI, INAF), it is now in advanced status of completion at INAF-Brera, Merate.[12] BEaTriX will generate a 17 cm × 6 cm parallel (≈ 2 arcsec) beam at either 1.49 keV or 4.51 keV. The beam will probe the SPO MMs that will be delivered from the production site, generating its X-ray focal spot on a CCD camera at a 12 m distance, and enabling the selection of the most performing modules to be aligned optically and integrated into the mirror assembly at the nearby company Media Lario.[13] The final mirror assembly of ATHENA will be ready for test and calibration at the VERT-X facility,[14] to be built next to the integration bench.

In this paper, we show the methodologies and the results of the simulations performed to assist the manufacturing of the optical components, with particular reference to the paraboloidal mirror, and so determine the expected performances of the final beam in terms of collimation, intensity, and uniformity. We briefly introduce the optical elements of BEaTriX in Sect. 2, even though a detailed description of the complete system can be found in another SPIE volume.[15] In Sect. 3, we provide a description of the metrological tools used to measure the paraboloidal mirror, the methods adopted for simulating its performance, and those of the entire system. In Sect. 4, we compare the mirror simulations with the experiment at PANTER. In Sect. 5, we describe the expanded beam we expect from metrology data. Sect. 6 provides a brief update on the wavefront sensing technique that will be used to align the paraboloidal mirror to the X-ray source.

2. THE BEATRIX X-RAY FACILITY

BEaTriX is a vacuum system consisting of two arms (Figure 1), approximately forming a right angle, fitting within a small lab (17 m × 8 m). The short arm generates, collimates, filters and expands the X-ray beam that will illuminate the SPO MM to be tested; the long arm enables the propagation of the focused beam over a 12 m range, out to the focal plane. The short arm will comprise two beamlines, one at 1.49 keV (the Al- Kα1 line) and another at 4.51 keV (the Ti- Kα1 line), while the long arm is in common for the two energies. To date, we have almost completed the 4.51 keV beamline, while the realization of the 1.49 keV beamline is envisaged to start soon.

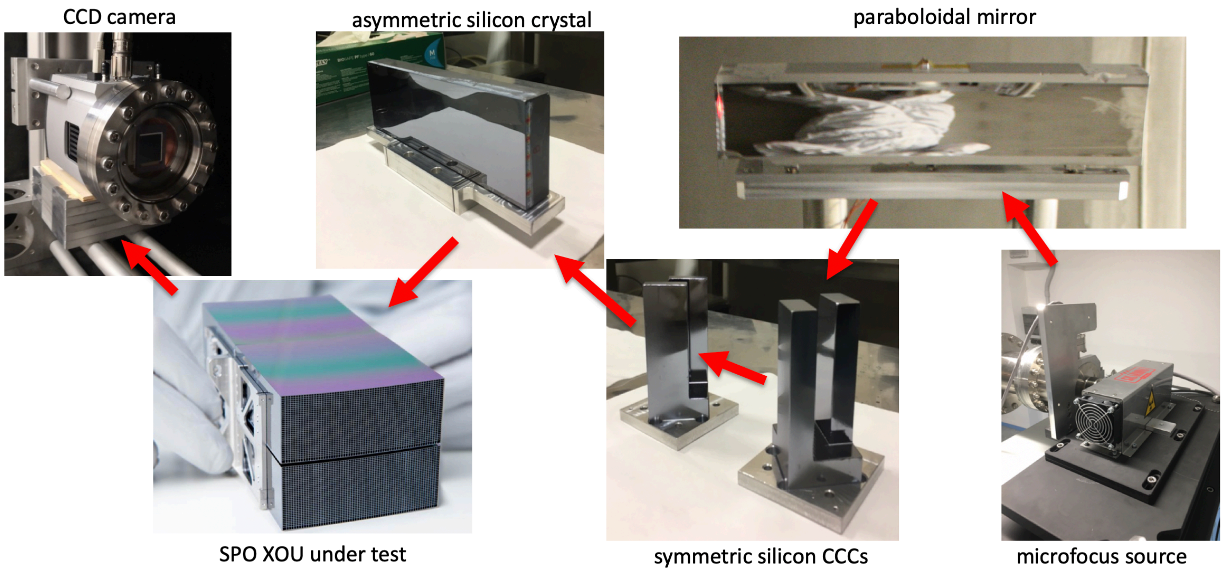

Figure 2: schematic of the optical chain in BEaTriX. X-rays are generated by an X-ray source with titanium anode (by Incoatec GmbH, Geesthacht, Germany) that uniformly illuminates a mirror in the shape of a paraboloid. The beam, now made parallel and expanded vertically to a 60 mm size, is spectrally filtered by a 4-bounce silicon monochromator (a pair of channel-cut crystals by Crystal Scientific Ltd, UK) to isolate a narrow portion of the Ti-Kα line. The monochromatic beam impinges onto the asymmetric crystal (by IMEM-CNR, Parma, Italy), which diffracts the beam at a nearly-right angle, expanding it horizontally to a 17 cm width. The beam then illuminates the aperture of an SPO MM or XOU, which forms its PSF on a CCD (provided by Andor Techn. Ltd.). Auxiliary components (vacuum pumps/gauges, beam monitors, slits, vacuum motors…) are not shown in this paper.

In the 4.51 keV beamline (Figure 2), the X-ray beam is generated by a microfocus source (a gaussian with 35 µm FWHM) with titanium anode, pre-collimated by a 400 µm diam. pinhole at a 2 cm distance. The source is located in the focus of a paraboloidal mirror at a 4.75 m distance, at the other end of the short arm, which makes the beam parallel and 6 cm tall. This paraboloid, pre-shaped by Zeiss, has been accurately polished and figured at INAF-Brera,[16] and coated at DTU with a 30 nm platinum layer to endow the mirror with reflection properties at 4.51 keV. A 4 nm chromium layer was deposited underneath the platinum to improve the coating adhesion. The following steps enable the horizontal expansion of the X-ray beam, exploiting the principle of diffraction by an asymmetrically-cut crystal.[17] Due to the dispersivity of asymmetric crystals,[18] however, the beam has to be made tightly monochromatic by a couple of channel cut crystals, mutually de-tuned in angle to narrow the spectral bandpass down to 30-50 meV.[19] The monochromatic beam is expanded horizontally to a 17 cm dimension by an asymmetric-cut silicon crystal, making it ready to illuminate the aperture of a MM. The focused beam is collected by a CCD, 12 m farther. In the 1.49 keV beamline, silicon crystals will have to be replaced by organic crystals (ADP),[20] which will require a separate setup.

All the optical components are enclosed in a system of vacuum tubes and chambers able to reach 10^{-6} mbar. The vacuum sections are partitioned by gate valves, in order to drastically abridge the time required for breaking and making the vacuum in the chamber that will house the MM. The long arm can be tilted to fit the reflection angle of the MM. All the components can be moved by precise vacuum motors and the entire system is controlled by dedicated software based on LabVIEW. The entire facility is built on building foundations to ensure its stability, and mounted on a heavy and damped anti-vibration platform made of reinforced concrete (Figure 3). More details on the configuration of the BEaTriX system can be found in a dedicated paper.[15]

Figure 3: the status of the BEaTriX lab in May 2020 (left) and in July 2021 (right). All the vacuum system was realized and installed by Kenosistec (Binasco, Italy) in a building basement and mounted on an anti-vibration platform. The chambers enclose the optical components that will expand and parallelize the X-ray beam. All the system fits within 17 m × 8 m.

3. MIRROR METROLOGY AND SIMULATION TOOLS

3.1. The mirror metrology tools (MPR and CCI)

The heart of the system is the paraboloidal mirror. The vertical divergence of the final beam essentially depends on the X-ray source size and is affected only by the transverse deviations of rays, which always have a lesser magnitude due to the incidence at a grazing angle. In contrast, the optical quality of the mirror is crucial in determining the horizontal collimation, the intensity, and the uniformity of the expanded beam. For this reason, a relevant effort has been devoted to polish and figure the paraboloid. The two tools used at INAF-Brera for taking the mirror within the prescribed specification are shown in Figure 4 and the finishing process are duly described in another contribution.[21] After every polishing or figuring iteration, the shape and the roughness of the mirror were accurately measured using the metrological tools available at Media Lario. This gave us feedback for the next iterations and allowed us simulating the expected performances of the expanded beam at every step of the surface working.

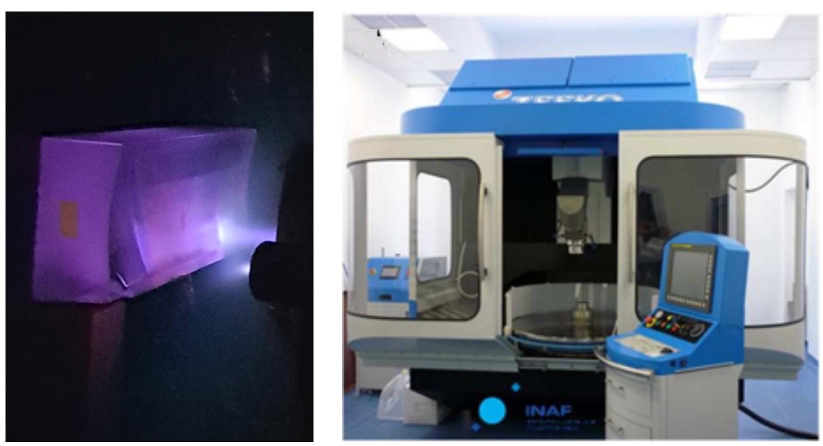

Figure 4: two steps in the manufacturing of the paraboloidal mirror at INAF-Brera. Left: Ion Beam Figuring for figure correction. Right: Zeeko IRP1200 polishing machine for roughness mitigation.

The metrology tools are the Mandrel Profilometer-Rotondimeter (MPR) and the CCI micro-interferometer, both operated at Media-Lario. MPR is a contactless and versatile shape detector,[22] developed in collaboration with LT Ultra Precision Technology GmbH. For measuring the BEaTriX mirror, an appropriate interface has been designed, and dedicated routines have been developed to reliably extract the error map, filtering the instrument dynamics out. The mirror has been characterized in the central 400 mm × 60 mm area (Figure 5, left), which fully encloses the beam involved in the asymmetric diffraction, at a 1 mm lateral resolution and a single-point vertical resolution of a few nanometers. CCI is a phase shift interferometer coupled to microscopes with magnifications 2.5×, 10×, 50×, developed by Taylor-Hobson. It returns 2D maps of the mirror surface microtopography, enabling assessment of the surface roughness. A 10× image of a surface's sampled point, in its final polishing state, is displayed in Figure 5, right. For both shape and roughness measurements, we note that residual defects and polishing marks have the same orientation as the optical axis; this minimizes their impact on the beam divergence in the horizontal plane. At the same time, owing to the incidence at a grazing angle of $\alpha = 0.91$ deg, ray deviations in the vertical plane are damped by a factor of $\tan\alpha = 0.0157$. In principle, only in-plane scattering could have been modeled from the longitudinal power spectral density, using the well-experienced 1D formalism.[23] Indeed, the marked anisotropy of roughness could make the out-of-plane scattering non-negligible, so we opted for a scattering modeling method in 2D (see next section).

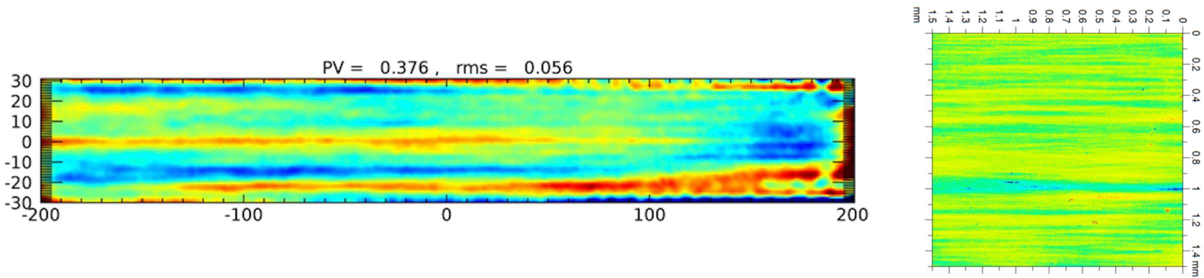

Figure 5: two typical metrological outputs for the BEaTriX paraboloidal mirror. Left: profile error map of the central 400 mm × 60 mm area of the collimating mirror surface, in its final manufacturing status, as obtained from the MPR at Media Lario; the optical axis is horizontal, vertical units are in microns. Right: a 10× image sampled on the mirror by the CCI micro-interferometer operated at Media Lario, RMS x: 5.1 Å, RMS y: 3.5 Å. The optical axis is aligned horizontally.

3.2. The BEaTriX mirror simulation

Two different codes were used for modeling the focus of the BEaTriX mirror. One is a conventional ray-tracing routine, taking as input the MPR map and the 2D scattering model derived from the CCI maps. A 2D scattering pattern is used to pseudo-randomly generate the in-plane and out-of-plane deviation angles, β and γ. We defer to Appendix A details about the inclusion of both deviation angles into a ray-tracing routine.

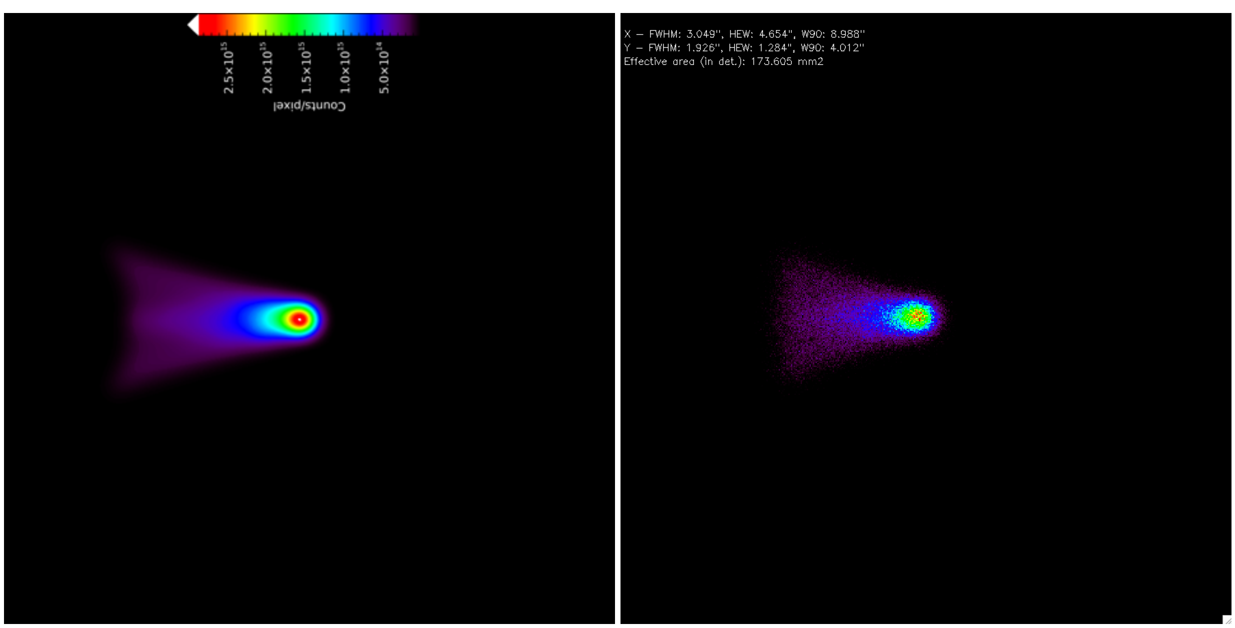

Figure 6: the simulated focal spot of the perfect paraboloid *in diverging X-ray illumination at PANTER. The best focus is located 200 mm farther from the source, with respect to the nominal focal distance. Even there, a small coma aberration remains, so a correction of the incident wavefront using a zone plate is necessary. The mirror faces the left side. Left: diffraction pattern at 1.49 keV from wavefront propagation. Right: result of a ray-tracing routine. The image sizes are 2 mm.*

The other simulation code computes the diffraction pattern from the OPD (optical path differences) introduced by mirror defects, misalignments, and the measurement setup, such as an X-ray source at a finite distance. For this code, we have used the same approach adopted in the SIMPOSIuM project to simulate silicon pore optics,[24] and in the VERT-X project to determine the alignment tolerances between the two segments of the Wolter-I collimator.[25] For instance, we show in Figure 6, left, the expected aberration at PANTER due to the very large, but finite, distance D of the X-ray source from the mirror aperture, at the nominal incidence angle α, even after re-adjusting the detector plane to the shifted best focus. The related OPD term is:

$$\Delta l_{\mathrm{D}} = \frac{x^2+y^2}{2D} + \frac{(x^2+y^2)x}{4D^2\tan\alpha\sin\alpha} \tag{1}$$

where x and y are the aperture pupil coordinates, with the origin in the mirror aperture center and the mirror facing left. The first term is the spherical aberration, easily corrected moving the focal plane at a distance f' fulfilling the relation $1/f' = 1/f - 1/D$. The second term generates the coma aberration, which can be removed only making the incident beam parallel; at PANTER, this can be done at 1.49 keV by means of a zone plate[26] as collimating optic. The expectations from the diffraction code and the ray-tracing code (Figure 6, right) exactly match each other.

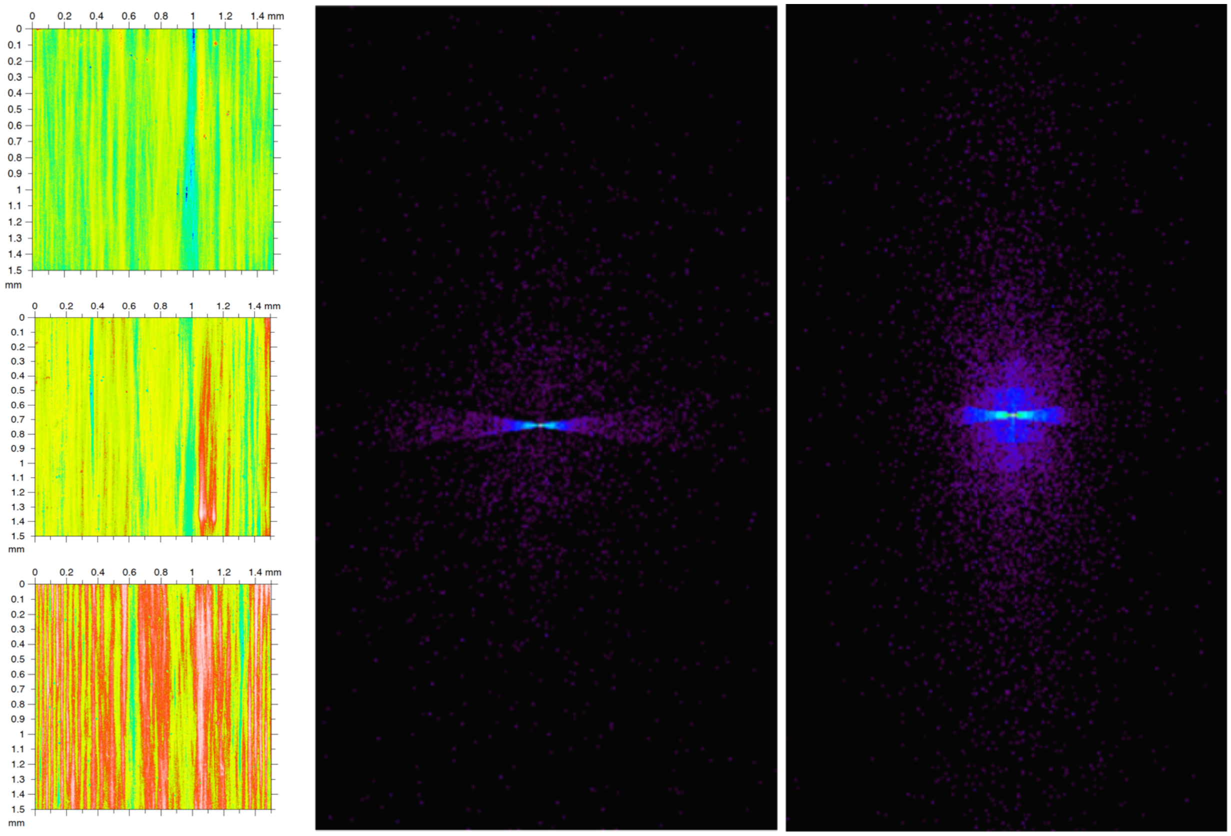

Figure 7: simulated diffraction pattern from mirror roughness. Left: a number of microtopography images taken on the BEaTriX mirror with CCI 10× have been stitched along the optical axis (in vertical) in order to obtain a 2D scattering diagram via the FFT of the complex pupil function (CPF). Center: expected diffraction pattern at 1.49 keV, HEW < 0.2 arcsec. Right: expected diffraction pattern at 4.51 keV, HEW < 0.5 arcsec. The color scale is logarithmic. The image widths are 18 arcsec.

As for the scattering component, the marked anisotropy of the roughness pattern requires computing the scattering distribution in 2D, directly using the 10× CCI microtopography maps as diffractive objects, projected along the line of sight, and taking the squared module of the Fourier transform of the phase shift map CPF.[24] Because the axial direction y is seen in projection in grazing incidence, a number of CCI maps were stitched together in a column to avoid contribution from aperture diffraction (along x, it is negligible as it is). The expected diffraction patterns at 1.49 keV and 4.51 keV are shown in Figure 7: as a consequence of the roughness directionality, even at a shallow angle incidence, X-ray scattering is preferentially *orthogonal* to the incidence plane. Anyway, at both energies, the scattering contribution to the HEW remains very small.