AHEAD Workpackage 8
JRA X-ray optics

Deliverable D8.1 – D35

Prototype Design and Performance Report

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1. INTRODUCTION

WP8 comprises 4 sub-work packages. These are being worked on in parallel

1) Optical design and optimization of X-ray optical systems. Includes all grazing incidence geometries: Wolter I, Kirkpatrick-Baez, Schmidt Lobster and Lobster Eye.

2) Assessment and modelling of inherent aberrations and error budgets for the technologies. A detailed breakdown and modelling of all the contributions which limit the angular resolution, size of field of view and collecting area.

3) Detailed simulation of instrument response for all cases. Prediction of the scientific performance.

4) Calibration and analysis of all cases. The measurement and subsequent analysis performance and calibration data taken from across the AHEAD consortium. Comparison of simulation with test data will inform the progress in points 1-3 above.

2. SIMULATION SOFTWARE qsoft

University of Leicester team: Richard Willingale, Vladimir Tichy

A PDRA, Vladimir Tichy, has been hired to work on AHEAD WP8 at The University of Leicester. He was due to start work on 22nd August 2016 but unfortunately suffered a serious back injury. Under medical advice he delayed his start to allow recovery from the injury and he eventually started work on 17th October 2016. Despite this delay we have made significant progress with setting up the first full version of the simulation software.

The package is called **qsoft** and comprises 5 modules

qfits	an interface to the HEASAC fitsio subroutine library
images	image manipulation, analysis and plotting
astro	astronomical and astrophysical applications
xsrt	X-ray sequential ray tracing
xscat	X-ray scattering, absorption and propagation

The first version of the software package is now running and has been installed on GitHub. The source can be obtained using git

```
git clone https://github.com/dickwillingale/qsoft.git
```

The applications are run as commands/functions within the scripting languages R and/or Python. The core code is written in Fortran and C which is compiled to produce shareable object libraries. The commands/functions are defined in R scripts or Python module scripts. The shareable objects are loaded by R or accessed as modules by Python. The qsoft collection should be built using the gcc and gfortran compilers. R and/or the Python module f2py must be available to create the shareable objects. Instructions to build qsoft are contained within the downloaded package. The system has been successfully tested under both the Linux and Mac OS-X operating systems.

We are now working on completing the full documentation. This is expected to be done in the next few months.

Sub-work package activities/progress

1) Optical design and optimization for different technologies

Silicon Pore Optics (as used for Athena)

The qsoft package includes a full simulation of the Athena mirror. The aperture contains >1000 SPO modules and each module is ray traced individually to produce the all-up mirror response. The axial curvature of each module can be specified to be: conical approximation, Wolter I curvature (1,1), Wolter I with spherical principal surface, a curved-plane combination (2,0) with a spherical principal surface, plane-curved combination (0,2) with a spherical principal surface, spherical principal surface with (-1/2,5/2) curvature ratio or (1/2, 3/2) (-1,3) (-1.5,3.5) (-2, 4) ratios.

The reflecting surface material composition and surface roughness power spectrum can be specified or tabulated reflectivity and scattering profile can be used.

The alignment and positioning errors of each module can be set. In-plane and out-of-plane figure errors can be specified for each module.

Detailed optical design of Silicon Pore Optics modules is in progress:

The impact of different wedge angle design options has been evaluated.

The impact of stray X-ray flux has been evaluated and the design and implementation of X-ray baffles investigated.

Detailed analysis of the angular resolution error budget (see below).

Micro Pore Optics (as used for wide field lobster eye modules)

The qsoft package can be used to simulate the performance of a lobster eye optic comprising a tessellation of square pore micro channel plates. The position and rotation of each plate within the aperture can be specified. At present the same pore size must be used for all plates but in the future, this will be changed so that it can be set for each plate individually. The thickness (pore length) of each plate can be set individually. A full set of plate/pore deformations can be specified for each plate including the intrinsic slumping errors, thermo-elastic distortions, pore axis pointing errors (plate bias errors), pore shear errors, errors associated with the multi-fibre structure in the plates and figure errors on the walls of the pores. The reflecting surface material composition and surface roughness power spectrum can be specified or tabulated reflectivity and scattering profile can be used.

The use of circular rather than square Micro Pore Optic elements for the lobster eye is under evaluation.

Kirkpatrick-Baez stacks (made by a modified version of the Silicon Pore Optics technology)

The qsoft package includes a simulation of tessellations of KB stacks made using SPO technology. SPO deformations and alignment errors for the KB stacks will be included in the future.

Schmidt Geometry lobster (using plane Si or glass plates)

Simulation of this geometry/technology is currently under construction within the qsoft package.

2) Assessment and modelling of inherent aberrations and error budget for the technologies

A detailed breakdown and modelling of all the contributions which limit the angular resolution, size of field of view and collecting area. A detailed model for the aberrations and error budget for both SPO and MPO Lobster eye is under development. Both models are now ready for testing against the measured response from the PANTER facility at MPE and similar facilities at the University of Leicester and GSFC in the US.

For example, the angular resolution error budget for the Athena SPO optics has 3 levels: SPO stack manufacture, SPO module performance, integrated system performance. These can be assessed by two methodologies: Root Sum Square of Half Energy Width contributions and detailed modelling of the PSF including all factor. The former is simple but approximate and includes no detailed PSF information. The latter provides and accurate physical representation with a PSF model as a function of energy and position in the field of view. It also incorporates the effective area and vignetting as a function of energy.

The qsoft package has been used to simulate the PSF of Athena SPO modules as illustrated in Fig. 1

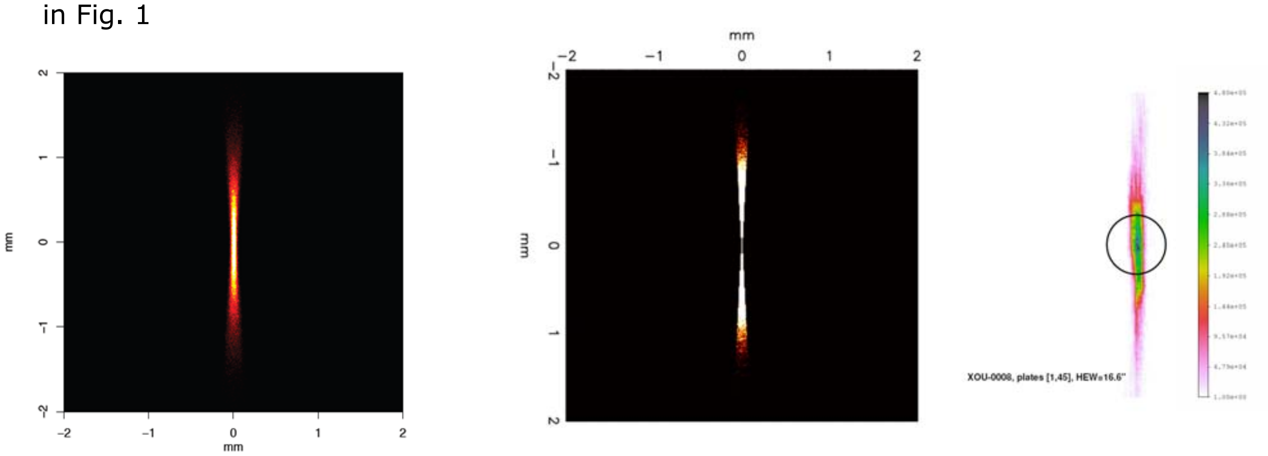


Figure 1: Left Athena SPO module PSF ray trace, middle in-plane errors only, right measured X-ray PSF

The extended elliptical distribution has a major axis dominated by in-plane errors and scattering from surface roughness and a minor axis introduced by out-of-plane errors, scattering and azimuthal curvature. The focal length error (axial offset from the optimum focus from the design value) arises from errors in the kink angle between the 1st and 2nd Si plate stacks and errors in the wedge angles within the plate stacks. Fig. 2 gives a breakdown of the contributions to the SPO modules RSS HEW error budget. Using qsoft we can ray trace the full complement of modules including realistic in-plane, out-of-plane errors, surface roughness for each module. We can confirm that a module HEW of 4.3 arc seconds can be achieved as indicated by the RSS calculation. We include module integration errors, dx,dy=0.03 mm rms for each axis, axial rotation errors of 3 arc secs rms. In addition, there will be gravity release errors allocated 1 arc sec HEW, thermal distortion errors allocated 1 arc sec HEW, moisture release allocated 1 arc sec HEW and mirror assembly tilt allocated 0.5 arc sec HEW.

- HEW error budget arc secs
  - RSS of in-plane and focal length errors
- Mirror plate errors - Figure 1.1
  Coating 0.5
  Roughness 0.6 1.3
- Mandrel 1.0
- Stacking - Confocal, wedge etc. 2.6
  - Local deformation dust 2.6 3.7
- Module assembly from 2 stacks 1.0
- Settling, creep 0.5
- Internal thermal distortion 1.0

- Total 4.3 arc secs

- Mandrel assumed to include axial curvature (Wolter I not conical approximation)

Figure 2 SPO module manufacture HEW error budget

Finally, we must include an allocation of 1 arc sec HEW for spacecraft pointing jitter and optical bench defocus. All this achieves an integrated system PSF performance of 5 arc seconds as required by the Athena specification.

3) Detailed simulation of instrument response for all cases: Prediction of the scientific performance

The qsoft package can be used to produce the predicted performance of the X-ray optics. For example, the Athena PSF as a function of off-axis angle and photon energy is illustrated in Fig. 3

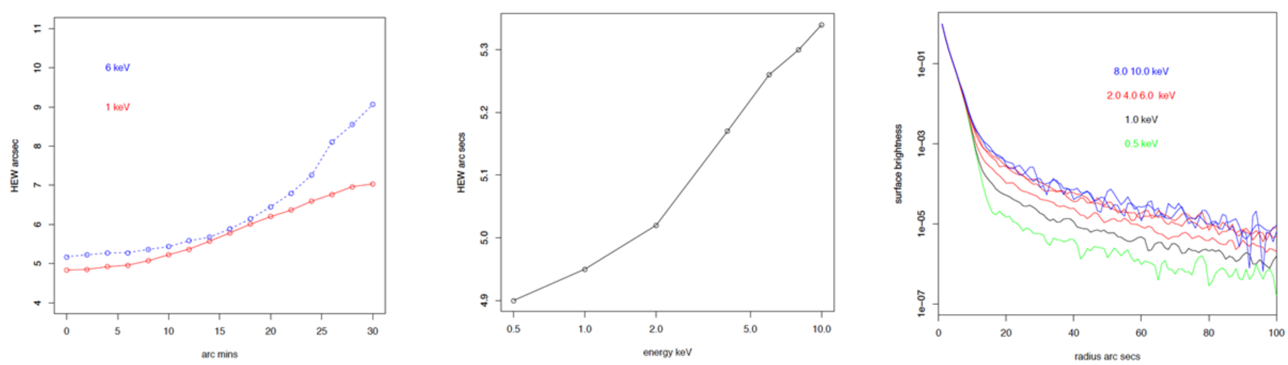


Figure 3: Athena PSF performance. Left the HEW as a function of off-axis angle at 1 and 8 keV. Middle the HEW as a function of energy. Right: the scattering wings as a function of energy.

The qsoft predicted PSF has been included in the Athena science simulator SIXTE which is under development at the University of Bamberg

http://www.sternwarte.uni-erlangen.de/research/sixte/index.php

4) Calibration and analysis of all cases: The measurement and subsequent analysis of performance and calibration data taken from across the AHEAD consortium. Comparison of simulation with test data will inform the progress in points 1-3 above.

The prototype software has been used to predict the high energy response of the Athena SPO mirrors in the energy range 10-30 keV for use in the evaluation of the cryogenic anticoincidence response for the X-IFY TES-array on Athena.

Initial tests of MPO optics and use of the qsoft analysis software has started. We have used the Leicester TTF to test a breadboard model of the SVOM MXT and the same model has been tested at the PANTER Test Facility. Both these test data sets have been analysed using the qsoft package developed under the AHEAD WP8.

We have demonstrated that the efficiency and angular resolution of the MPOs can be reliably extracted from the test data. We have demonstrated that there is a good agreement between the data obtained at the Leicester TTF and PANTER.

Fig 4 shows an X-ray exposure produced using a single MPO on the SVOM MXT breadboard in the Leicester TTF.

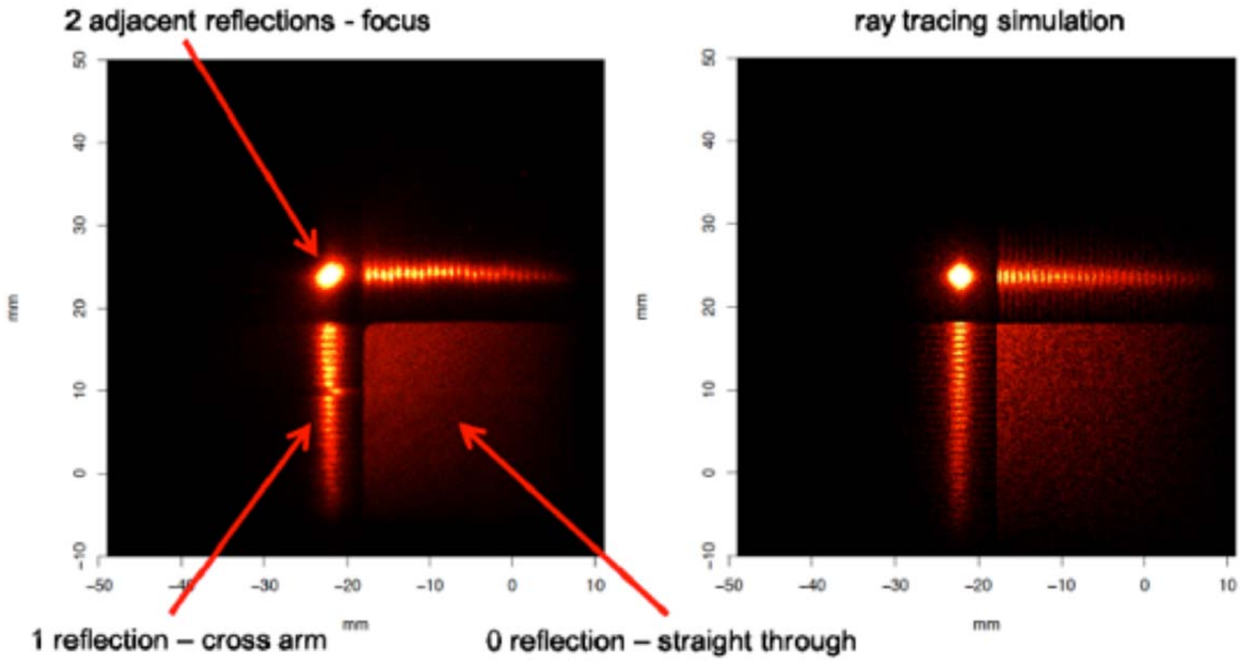


Figure 4. Left: 1.5 keV X-ray exposure using a single MPO. Right: simulation of the exposure using qsoft.

The source is off-set from the axis at the centre of the plate such that the focused spot appears outside the straight through patch. All 3 PSF components from the lobster eye are seen separated in the image so the exposure is self-calibrating. The distance from the shadow corner of the straight through patch and the focused spot gives the angular position of the source and comparison of the brightness in the straight though patch and the focused spot can be used to give the efficiency of the plate. Fig. 5 shows the horizontal and vertical profiles along 1 mm wide strips through the focused spot and 1 reflection cross-arms in Fig. 4. The simulated profiles match the measurements in detail. The modulation of flux in the cross-arms is produced by the multi-fibre structure within the MPO. The focused spot has a Gaussian profile core produced by pore within the central regions of the multi-fibres but broader wings result from larger pore tilt and figure errors around the perimeter of the multi-fibres. A careful comparison between the measured and simulated data enables us to quantify the aberrations and distortions within the MPOs.

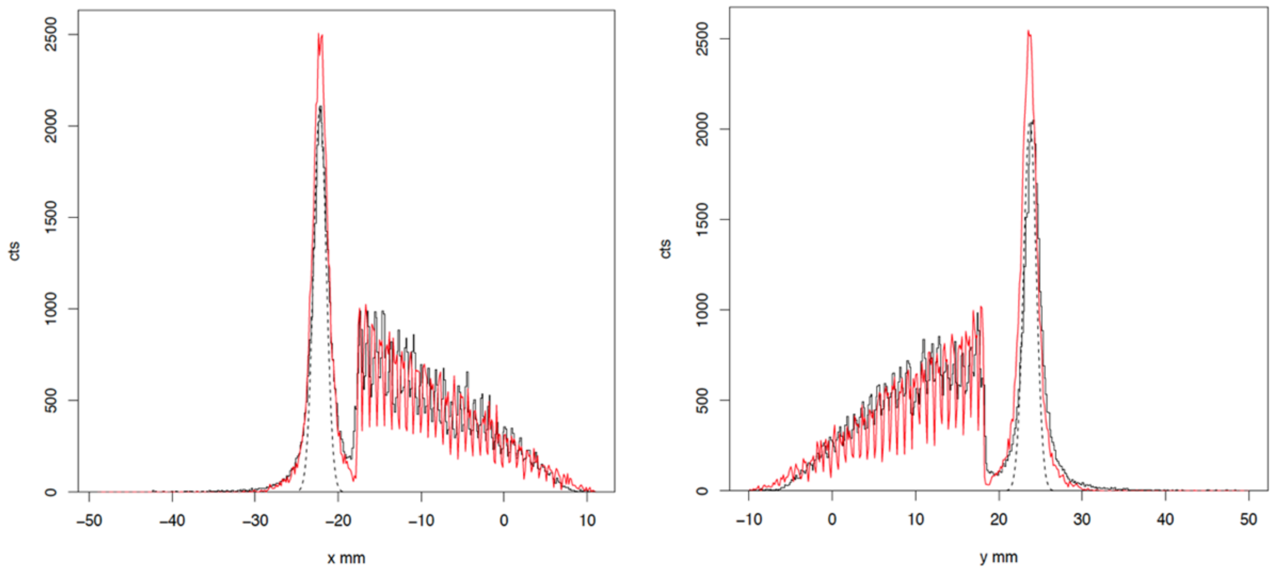
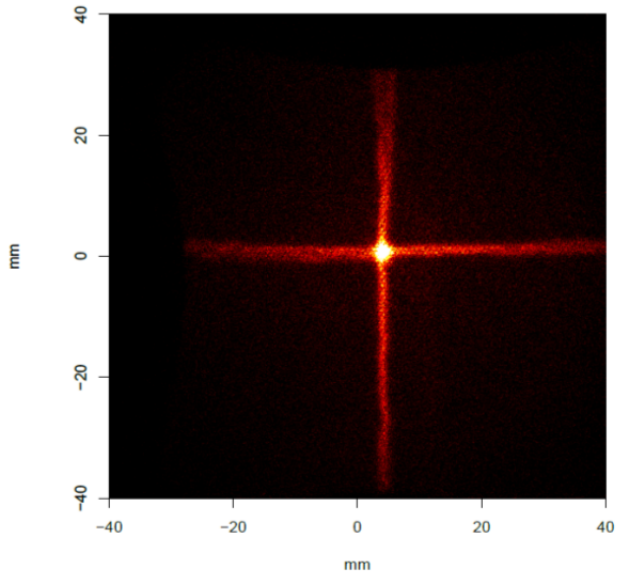


Figure 5: Horizontal and vertical profiles through the images in Fig. 4.

The same software has also been used to analyse data from the long beam line X-ray test facility at GSFC facility at GSFC. This has provided another very useful source of results on the angular resolution and efficiency of MPOs with a smaller radius of curvature to those tested at Leicester and PANTER and with a coating of Platinum rather than Iridium.

At Leicester, we have started a new campaign of X-ray testing looking at the performance of square pore MPOs at different stages of their manufacture. By doing this we hope to be able to pinpoint the critical manufacturing processes that are limiting the performance. Fig. 6 shows an image produced from a bare glass square pore MCP tested flat, prior to slumping, in a point-to-point focusing mode. The match between the measured data and simulation is good although there is clearly some extra spreading of flux in the cross-arms not accounted for by the current simulation. The FWHM of the focused spot is 6.95 arc mins and the efficiency of the plate wrt to that expected from the bare glass is 81%. Because this plate was tested before slumping we know that the angular resolution performance is limited by the pore quality in the multi-fibres produced by the initial fusing of the glass and etching process and not the slumping process used to bend the plate into the spherical form required for imaging a source at infinity. We hope to perform further tests when the same plate has been slumped and then after it has been coated with Iridium. The qsoft package being developed under the AHEAD work is crucial in this test campaign and the results will be used to inform and improve the software model of the aberrations and distortions within the MPOs.



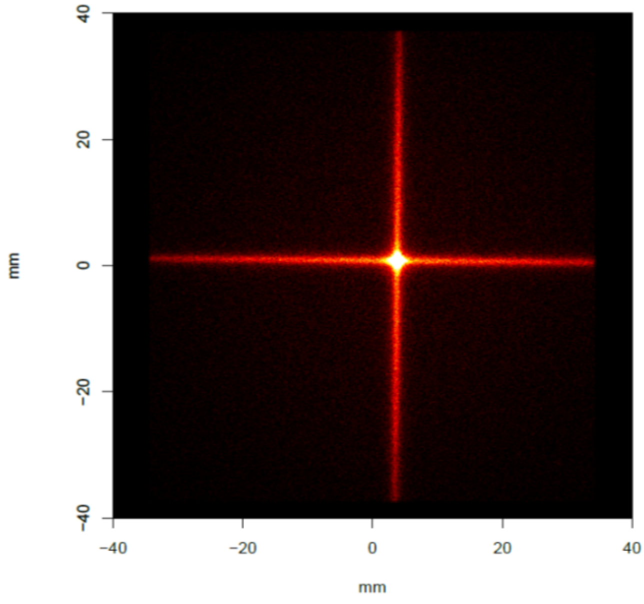


Figure 6: Point-to-point X-ray imaging test of a flat square pore MCP. Left: the response measured at 1.5 keV. Right: the predicted response produced by qsoft.

3. Kirk Patrick Baez Optics

CTU Prague project team / report authors: Veronika Maršíková, Adolf Inneman, René Hudec

Introduction

The goal was to design X-ray optics module in Kirkpatrick Baez (KB) arrangement for test experiment at the PANTER facility of the MPE (Max-Plank-Institut für Extraterrestrische Physik). X-ray optics module of Kirkpatrick Baez (KB) geometry was designed with respect to real experiment. After that, detailed simulation was performed and is reported here. The simulations take into account manufacturing constraints.

Design

X-ray optics type KB was proposed for X-ray tests at PANTER facility. The X-ray optic is composed of two 1D sub-modules. Both sub-modules are assembled from 2D parabolic reflective foils. The sub-module A is more distant from detector and foils are in vertical arrangement. The sub-module B is closer to detector and foils are in horizontal arrangement.

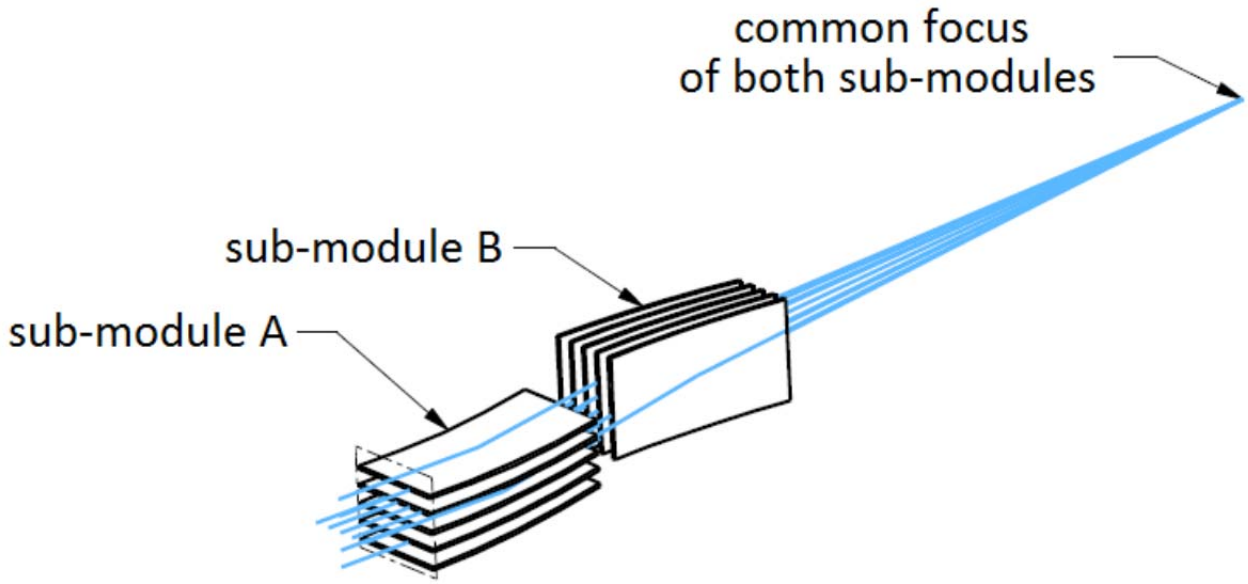


Figure 1: X-ray optics type Kirk-Patrick Baez (KB) – both sub-modules have common focus.

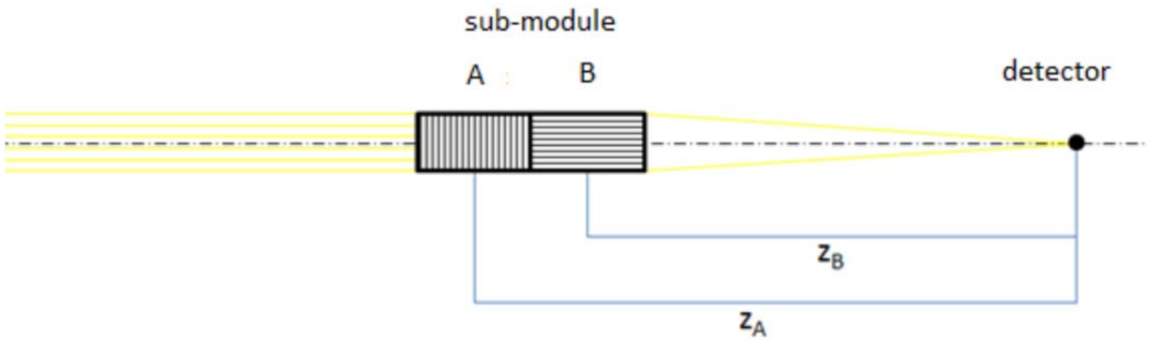


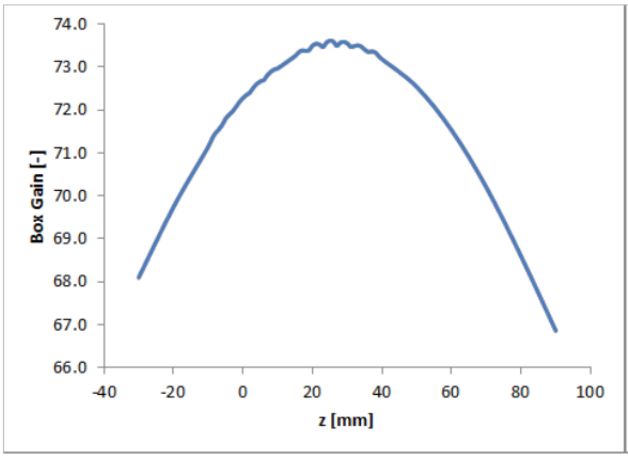
Figure 2: Experimental setup proposed for testing a Kirk Patrick-Baez (KB) optic at PANTER.

Table 1: Parameters for simulation

Table 1: Parameters for simulation Number of foils	10
Dimension of foils	100 x 100 x 0.4 mm
Spacing	7 - 8 mm
Reflective surface	Au
Dimension of modules	100 x 25 x 300 mm
Aperture	100 x 20 mm
Focus zA/zB	7 155 /6 825 mm
Source	endlessly
Detector	512 x 512
Pixel size	37.5 μm

In the first step, optimal position of each module was investigated. Then, both sub-modules were positioned in the ideal place and ray-tracing of X-ray optics was done for different energy i.e. for ideal case (reflection 100%), for reflection 50% and for energies from 110 eV to 4 500 eV.

1D sub-modules



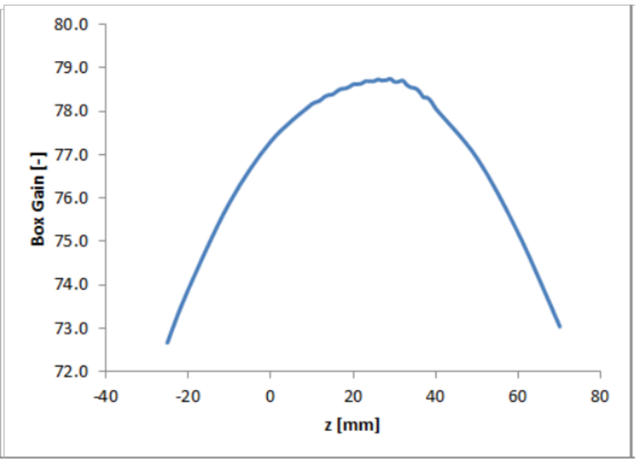


Figure 3: Looking for optimal position for 1D module A (left) and 1D module B (right) – dependence of gain in focus on detector position.

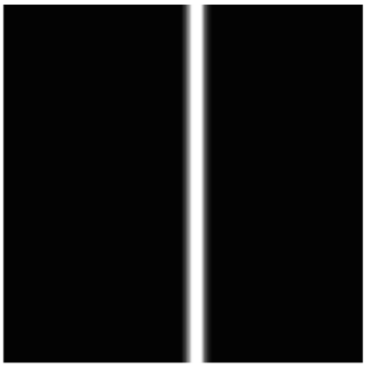


Figure 4: Ray-tracing simulation of 1D LE optics for sub-module A (left) and sub-module B (right) for source-detector distance of 7 m for ideal mirrors, ideal position.

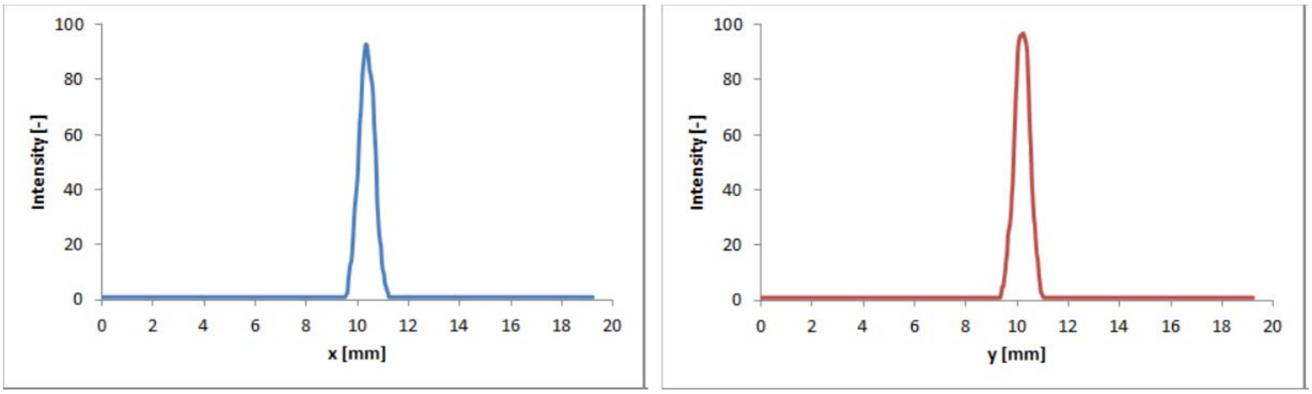


Figure 5: X-axis (left) and Y-axis line profile of image data summed from detector pixels.

Table 2: Results from ray-tracing for sub-module A and B (ideal mirrors):

	Sub-Module A	Sub-Module B
FWHM [μm]	725.5	705.7
G [1]	75.2	80.5
ω [arcsec]	21.4	20.8

G – gain, ω – angular resolution

2D optic (sub-module A and sub-module B):

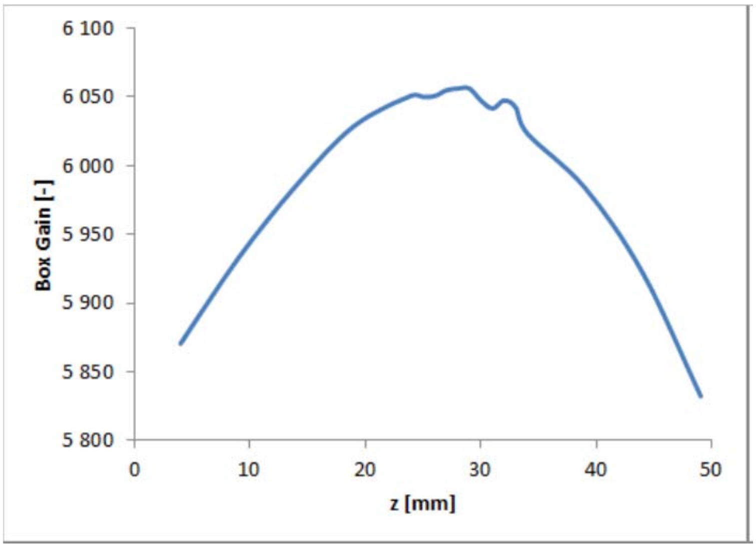


Figure 6: Looking for optimal position of 2D X-ray optics – dependence of gain in focus on detector position.

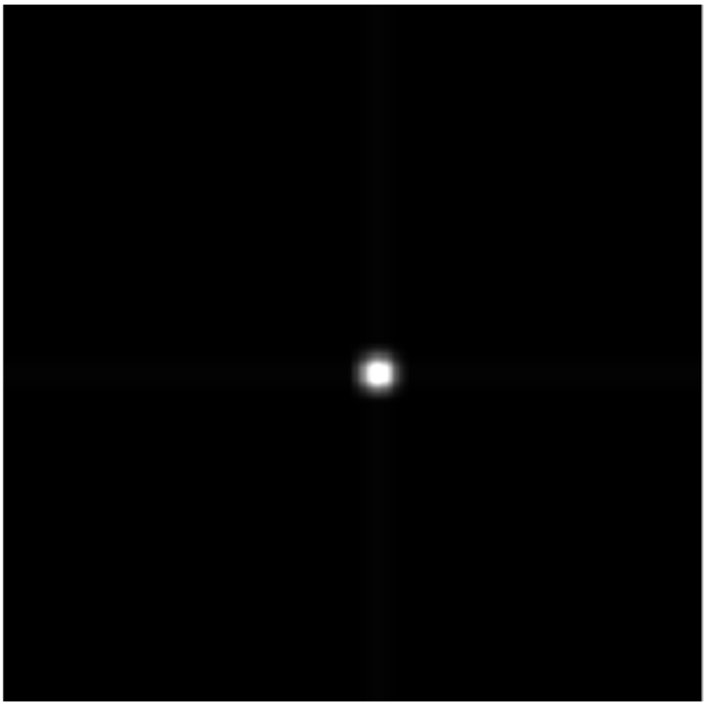


Figure 6: Ray-tracing simulation of 2D X-ray optics for source-detector distance of 7 m for ideal mirrors.

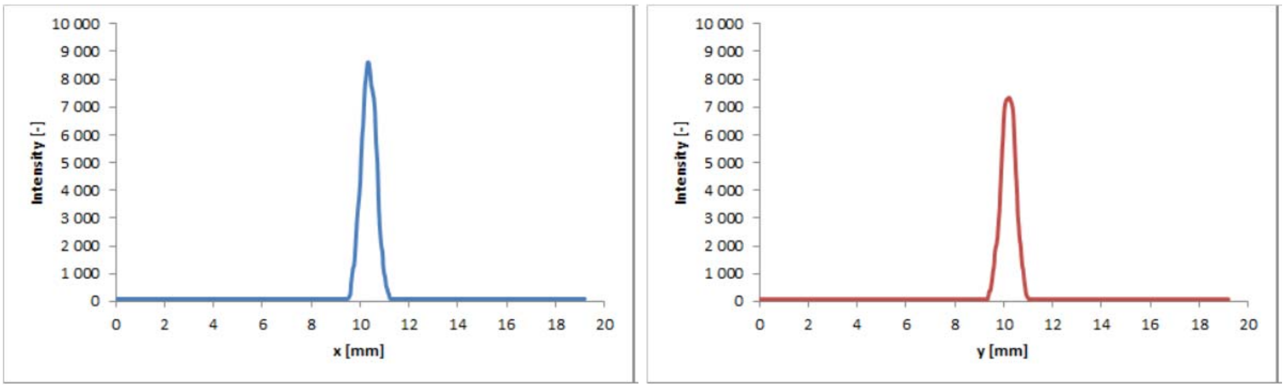


Figure 7: X-axis (left) and Y-axis line profile of image data summed from detector pixels.

Table 3: Results from ray-tracing for whole X-ray optic (ideal mirrors):

	vertical	horizontal
FWHM [μm]	725.5	705.7
G [1]	6 054	
ω [arcsec]	21.4	20.8

Table 4: Energy – X-ray emission Lines

Be Ka1	110 eV
C Ka1	277 eV
Ti La1	453 eV
Cu La1	930 eV
Al Ka1	1 487 eV
Au Ma1	2 123 eV
Pd La1	2 839 eV
Ti Ka1	4 511 eV

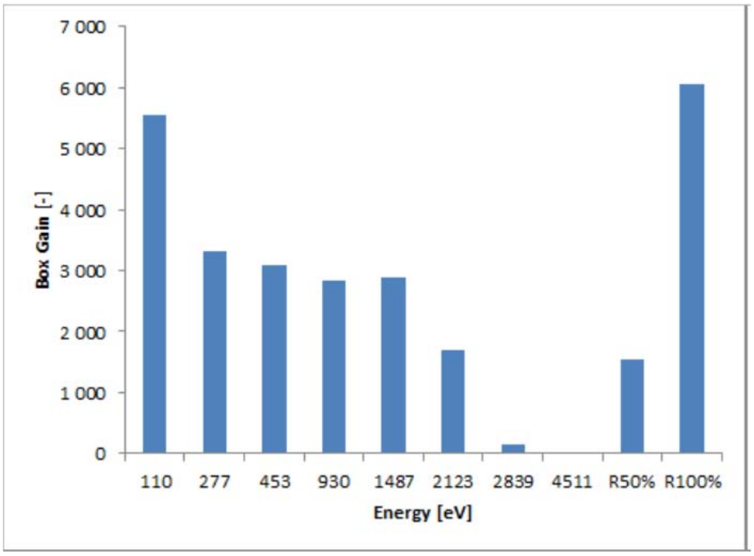


Figure 8: Dependence of gain in focus on energy.

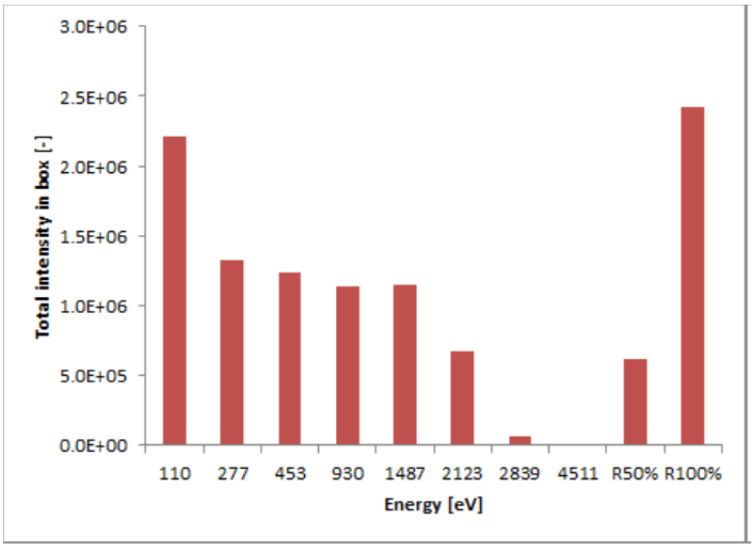


Figure 9: Dependence of the intensity in focus on energy.

The large difference between energy 2 123 eV and 2 839 eV is due to absorption M-edge for gold. Surface of foils can be coated by different material and then X-ray optics can be used at higher energy (for example iridium or ruthenium).

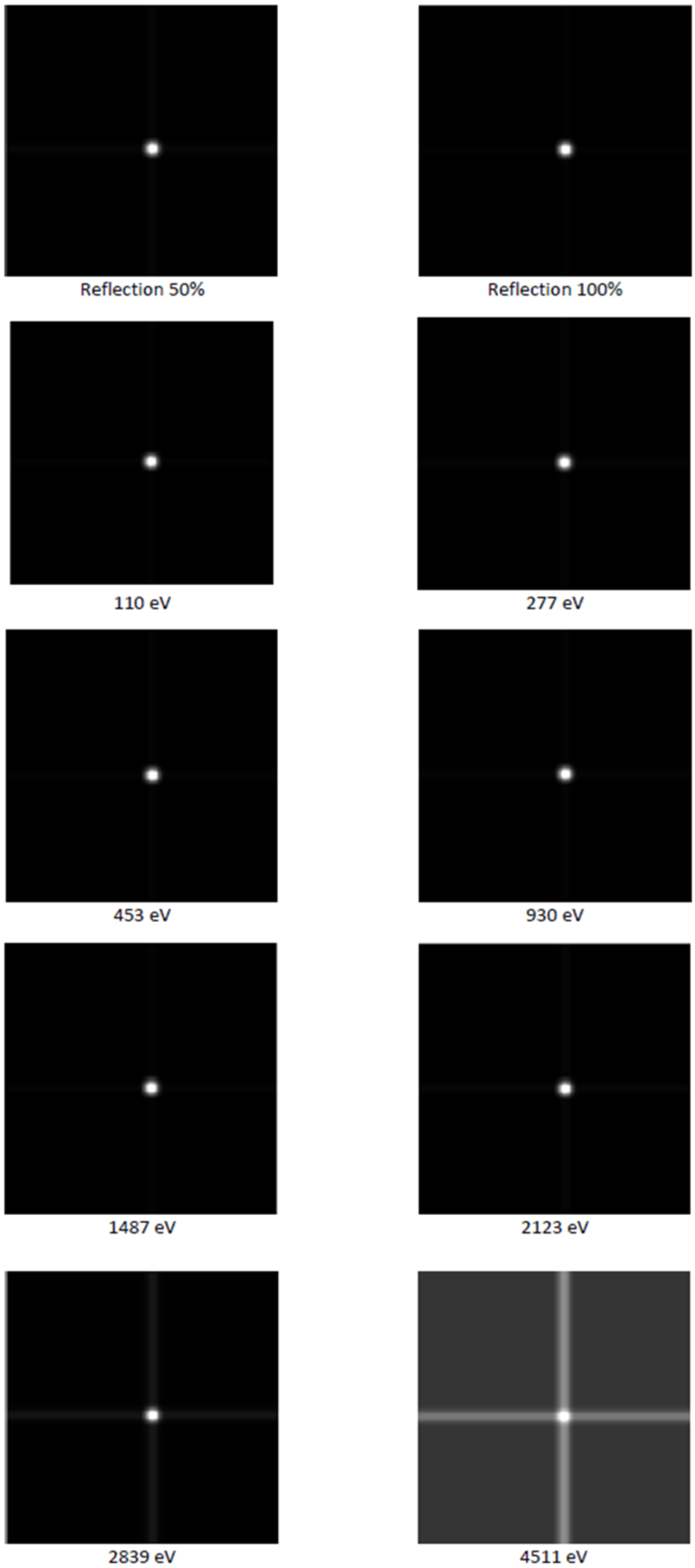


Figure 10: Ray-tracing simulation of 2D LE optics for source-detector distance of 7 m for various energies.

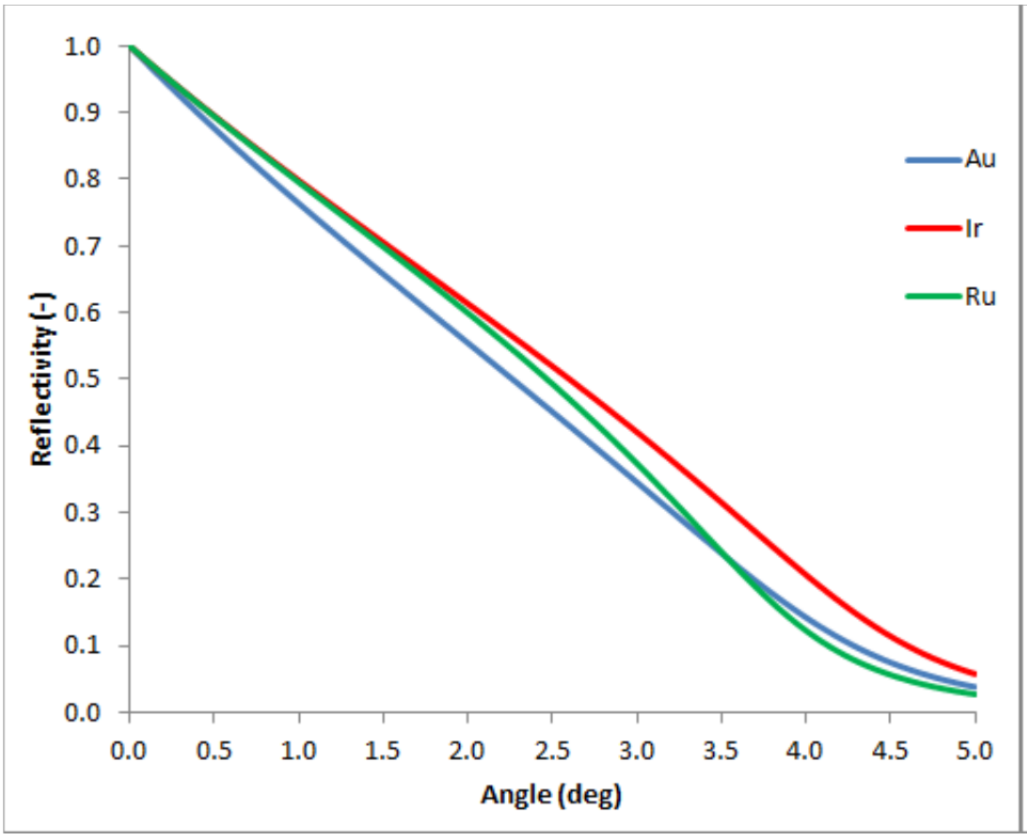


Figure 11: Comparison of various surface materials (gold, iridium and ruthenium) – dependence of reflectivity on angle.

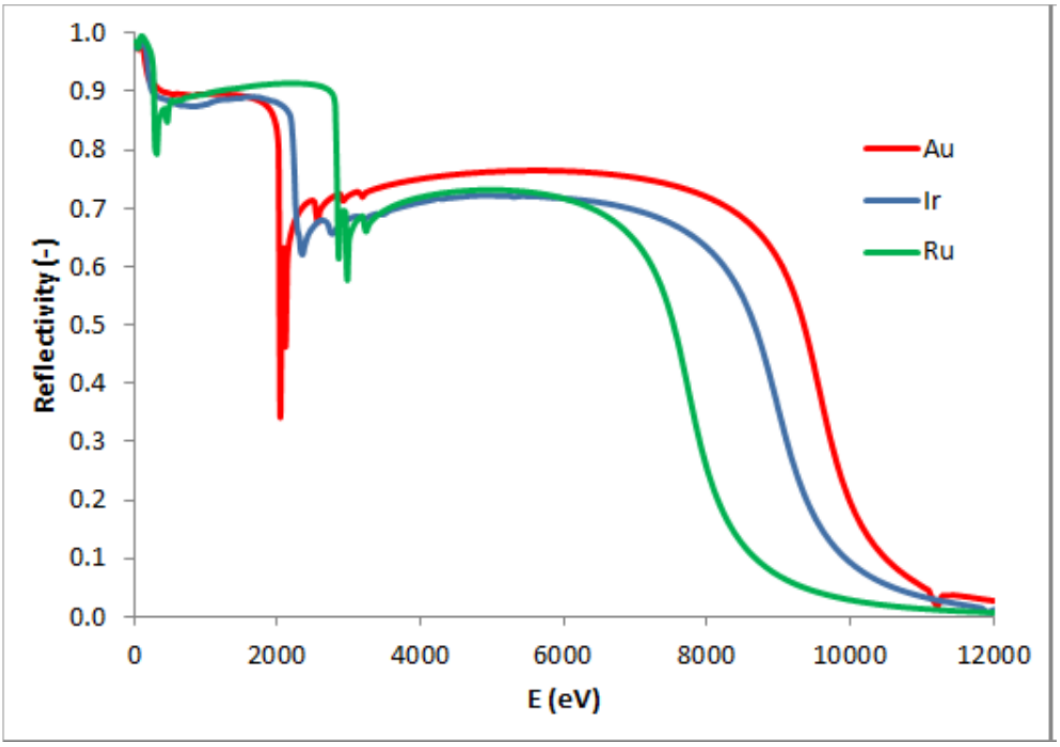


Figure 12: Comparison of various materials (gold, iridium and ruthenium) – dependence of reflectivity on energy.

Results

KB X-ray optics module for PANTER tests was designed and studied. X-ray optics test module will be prepared based on this study. Skeleton of optic will be prepared from titanium and foils will be with Au surface. We plan to prepare 2 types of optics modules – one with glass foils and second with silicon foils. We plan to test first one in January 2017.

Used parameters/symbols:

G – gain
ω – angular resolution
Box – square area around focus
Box Gain – gain in focus
Intensity in box – total intensity in focus

4. REFERENCES

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