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Authors	Ferreira, Desiree D. M.; Knudsen, Erik B.; Westergaard, Niels J.; Christensen, Finn E.; Massahi, Sonny; et al.
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Simulating X-ray telescopes with McXtrace: A case study of ATHENA's optics

Desiree D. M. Ferreira[a], Erik B. Knudsen[b], Niels J. Westergaard[a], Finn E. Christensen[a], Sonny Massahi[a], Brian Shortt[c], Daniele Spiga [d], Mathias Solstad[e], Kim Lefmann[e]

[a]DTU Space, Technical University of Denmark, Elektrovej, bygn. 327, 2800, Kgs. Lyngby, Denmark
[b]DTU Fysik, Technical University of Denmark, Fysikvej, bygning 311, 2800, Kgs. Lyngby, Denmark
[c]European Space Agency (ESTEC), Keplerlaan 1, PO Box 299, 2200 AG, Noordwijk, Netherlands
[d]INAF - Osservatorio Astronomico di Brera, Via E. Bianchi 46, Merate (LC), Italy I23807
[e] Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100, Copenhagen, Denmark

ABSTRACT

We use the X-ray ray-tracing package McXtrace to simulate the performance of X-ray telescopes based on Silicon Pore Optics (SPO) technologies. We use as reference the design of the optics of the planned X-ray mission Advanced Telescope for High ENergy Astrophysics (ATHENA) which is designed as a single X-ray telescope populated with stacked SPO substrates forming mirror modules to focus X-ray photons. We show that is is possible to simulate in detail the SPO pores and qualify the use of McXtrace for in-depth analysis of in-orbit performance and laboratory X-ray test results.

Keywords: ATHENA, ray tracing, McXtrace, simulation, X-rays, SPO, effective area, mirror module

1. INTRODUCTION

The aim of this study is to demonstrate the use of McXtrace[1] to simulate the performance of X-ray telescopes. Our goal is to realistically simulate the X-ray optics taking into consideration all known physical processes affecting the performance of the telescope.

McXtrace is a open source Monte Carlo software package for simulating x-ray optics and performing virtual X-ray experiments. It was developed with the main objective of supporting optimisation of X-ray beam lines and is now used in several setups such as data analysis and experiments. McXtrace allows for modular simulations where each pore within a SPO mirror module can be traced and simulated.

We take advantage of the available database of X-ray elements already included in the McXtrace[1] package to build a ray tracing model of the ESA's next large X-ray mission called Advanced Telescope for High ENergy Astrophysics (ATHENA).[2] The ATHENA mission has its launch foreseen in 2028 and will address to two key astrophysical questions: "How does ordinary matter assemble into the large-scale structures we see today?" and "How do black holes grow and shape the Universe?".[2]

ATHENA will consist of a single X-ray optical module with a 12 m focal length. The two instruments onboard are the X-ray Integral Field Unit (X-IFU)[3] and the Wide Field Imager (WFI).[4]

ATHENA's optics is based on Silicon Pore Optics (SPO) technology.[5–8] So far we have implemented a simulation of the baseline geometry and mirror coatings, a Wolter-I X-ray optic with a radius of 1.5 m populated with SPO mirror modules coated with an Ir/B_4C bilayer.

The Wolter-I telescope consists of a confocal and coaxial paraboloid and hyperboloid mirrors. X-rays reach the paraboloid mirror at small grazing angles, and are focused after being are reflected first by the paraboloid mirror then by the hyperboloid mirror.[9,10] Figure 1 illustrates the double reflection and focused rays.

As the study and optimisation of the geometry of the optics evolve we will implement and simulate other geometries.[11] Ray-tracing with McXtrace is done on individual pore level and allow for evolution to a single SPO mirror plate, mirror modules and the complete ATHENA setup.[12–14]

Further author information:
Send correspondence to:
Desiree Della Monica Ferreira, e-mail: desiree@space.dtu.dk

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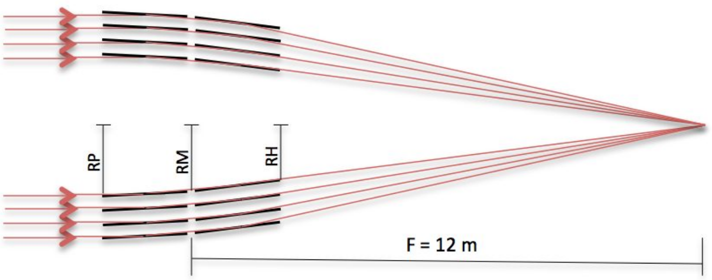

Figure 1. Schematic drawing showing the parabolic and hyperbolic set of mirrors for a Wolter I geometry allowing for double reflection and focussing. The parabolic radius (RP), hyperbolic radius (RH) and mid radius (RM) are indicated.

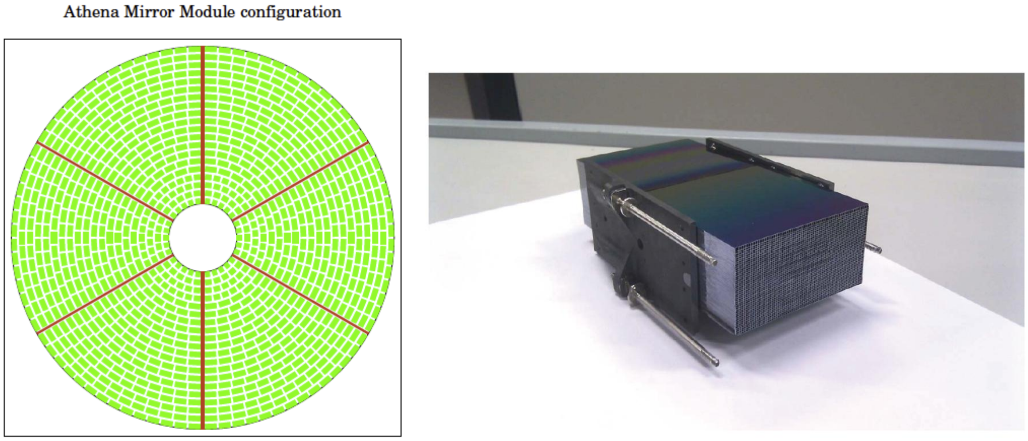
Athena Mirror Module configuration

Figure 2. Left: Illustration of the present geometry of ATHENA's optics showing the distribution of mirror modules within the optics (177 mirror modules per petal, 6 petals). Right: Example of a SPO mirror module. Here we observe the SPO plates stacked to form the reflecting pores (image credit: ESA).

2. ATHENA GEOMETRY BASED ON SPO

We simulate a telescope geometry that closely match the actual ATHENA design, described in this section. We start from the baseline configuration of a Wolter I profile. The pore geometry reproduces the SPO design and positions of each mirror module. The geometry of each mirror module varies according to its radial position in the optical module. The distribution of mirror modules within the optical module is illustrated in figure 2. Table 1 lists the length and width of the SPO plates within a mirror module row along with the parabolic (RP), hyperbolic (RH) and middle (RM) radius at the centre of each of the 20 mirror module rows (considering plate 34 (pl34) to be the central reflecting plate in a mirror stack of 68 reflecting mirror plates). RP, RM and RH are also indicated in figure 1. The dimensions assumed for the pore geometry and baseline coating of Ir/B4C are represented in figure 3.

A summary of the present ATHENA's geometry is shown in table 2. The incident grazing angle α at the

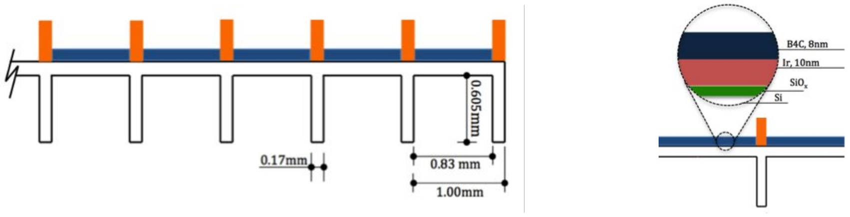

Figure 3. Schematic drawing showing the dimensions assumed for the pore geometry and baseline coating of Ir/B4C.

Row	Length (m)	RH pl34 (m)	RM pl34 (m)	RP pl34 (m)	Width (m)
1	0.101504	0.282022	0.283822	0.284423	0.037096
2	0.083388	0.344215	0.346017	0.346618	0.050159
3	0.070762	0.406408	0.408212	0.408814	0.049839
4	0.06146	0.468602	0.470407	0.471009	0.049614
5	0.054321	0.530796	0.532603	0.533205	0.089363
6	0.048671	0.59299	0.594798	0.5954	0.082476
7	0.044087	0.655185	0.656993	0.657595	0.077572
8	0.040294	0.717379	0.719188	0.71979	0.086892
9	0.037104	0.779574	0.781383	0.781986	0.082053
10	0.034383	0.841769	0.843578	0.844181	0.090205
11	0.032036	0.903963	0.905773	0.906376	0.085538
12	0.02999	0.966158	0.967968	0.968571	0.092783
13	0.028191	1.028353	1.030163	1.030766	0.088327
14	0.026597	1.090548	1.092357	1.092961	0.094845
15	0.025175	1.152743	1.154552	1.155156	0.090609
16	0.023898	1.214938	1.216747	1.217351	0.08708
17	0.022746	1.277133	1.278942	1.279546	0.09251
18	0.0217	1.339328	1.341137	1.341741	0.089107
19	0.020748	1.401523	1.403332	1.403936	0.09412
20	0.019876	1.463718	1.465527	1.466131	0.090845

Table 1. Input parameters for each mirror module row considered for ray tracing. Row number, SPO plate length, radius at the end of the hyperbolic mirror plate (RH), radius between the hyperbolic and parabolic plate (RM), radius at the beginning of the parabolic plate (RP), SPO plate width .

centre of each mirror module row is computed following a conical approximation of a Wolter I geometry and is given by

$$\tan 4\alpha = \frac{r}{F_L} \quad , \tag{1}$$

where F_L is the focal length (12 m) and r the radius, in this case considered to be the mid radius (RM). The projected area is calculated by multiplying the area of one single pore by the number of pores within a mirror module and by the number of mirror modules in each row. The baseline coating of the ATHENA mirrors is a single bilayer of Ir/B_4C and the reflectivity at 1 keV for the row incident grazing angle is obtained using the IMD software.[15] The on-axis effective area A_{eff} is computed assuming

$$A_{eff} = \sum_{i=1}^{n_p} A_p \cdot R(E,\alpha)^2 \quad , \tag{2}$$

where A_p is the mirror plate pore area, R(E,α) is the mirror reflectivity, and n_p is the total number of pores for all reflecting mirror plates. For a more detailed description of the effective area calculation see e.g.[6, 16, 17]

3. MCXTRACE SETUP

McXtrace,[1] is a general Monte Carlo ray tracing software package for performing simulations of X-ray optics and experiments.[18–20] Due to its very modular open structure it is particularly well suited to the situation with the ATHENA's optics, where each SPO may be evaluated individually. As the project is in a phase where various optical designs are being considered this is a major advantage.

McXtrace utilises the principle of a Domain Specific Language (DSL), i.e. the optical setup of an instrument, e.g. telescope, is described in a special language, giving optical parameters and spatial coordinates for (at least) the significant devices in the optical setup.

ring	grazing angle (^{o})	number of MM	projected area (m^2)	reflectivity at 1 keV	on-axis A$_{eff}$ at 1 keV (m^2)
1	0.341	30	0.038	0.973	0.0357
2	0.416	30	0.051	0.965	0.0477
3	0.490	36	0.060	0.959	0.0553
4	0.564	42	0.070	0.952	0.0637
5	0.638	30	0.091	0.945	0.0815
6	0.713	36	0.101	0.939	0.0888
7	0.787	42	0.110	0.931	0.0958
8	0.861	42	0.123	0.924	0.1053
9	0.935	48	0.134	0.916	0.1128
10	1.010	48	0.147	0.908	0.1216
11	1.084	54	0.157	0.899	0.1268
12	1.158	54	0.170	0.890	0.1346
13	1.232	60	0.180	0.881	0.1401
14	1.307	60	0.193	0.871	0.1463
15	1.381	66	0.203	0.861	0.1504
16	1.455	72	0.214	0.850	0.1545
17	1.529	72	0.226	0.838	0.1588
18	1.604	78	0.237	0.825	0.1613
19	1.678	78	0.250	0.811	0.1646
20	1.752	84	0.258	0.795	0.1633

Table 2. Summary of ATHENA's performance at 1 keV. Angles, reflectivities and areas.

This description is automatically translated into a computer program in the C-language,[21] which may be compiled and executed on the target platform which is to run the simulations. This procedure has a couple of advantages:

1. The executable can be optimised by the compiler for the target platform.
2. The simulation code contains only the code actually used. A simulation of a telescope will not contain code describing the inner workings of a synchrotron undulator.[22]
3. Since it is c-based, the optics description may be extended at will by including C-code directly in the description.

Any McXtrace device, denoted *component*, corresponds to an independent structured file containing C-code. In essence, this piece of code describes the interaction of a single X-ray with the component in the coordinate frame of the component. The McXtrace system then takes care of coordinate transforms between frames and X-ray transport between components. As a result, the component codes generally get clear logical boundaries, making each piece of component code small and manageable. As an example, the code written specifically for ATHENA modelling of a single parabolic SPO pore is < 400 lines, including documentation.

Originally designed for simulations of X-ray scattering experiments at large scale facilities, McXtrace is equally applicable to any situation where a general optical beam path is to be followed. To evaluate the performance of ATHENA, a (small) set of new components had to be written to describe the SPO. Pore size, focal length, etc. are simply parameters that can be changed at will. One upshot of the modular structure of McXtrace, of interest for the ATHENA telescope mission, is that the SPO may easily be inserted into a completely different surrounding setup. This enables us to model the response expected when the SPOs are tested and characterised e.g. at the laboratory of PTB at BESSY II in Berlin.[23, 24]

In this simulation effort we have chosen the single SPO pore as a building block, as it allows full flexibility in the design process, when many different optical designs have to evaluated. Thus the parameters of every single pore may be specified independently.

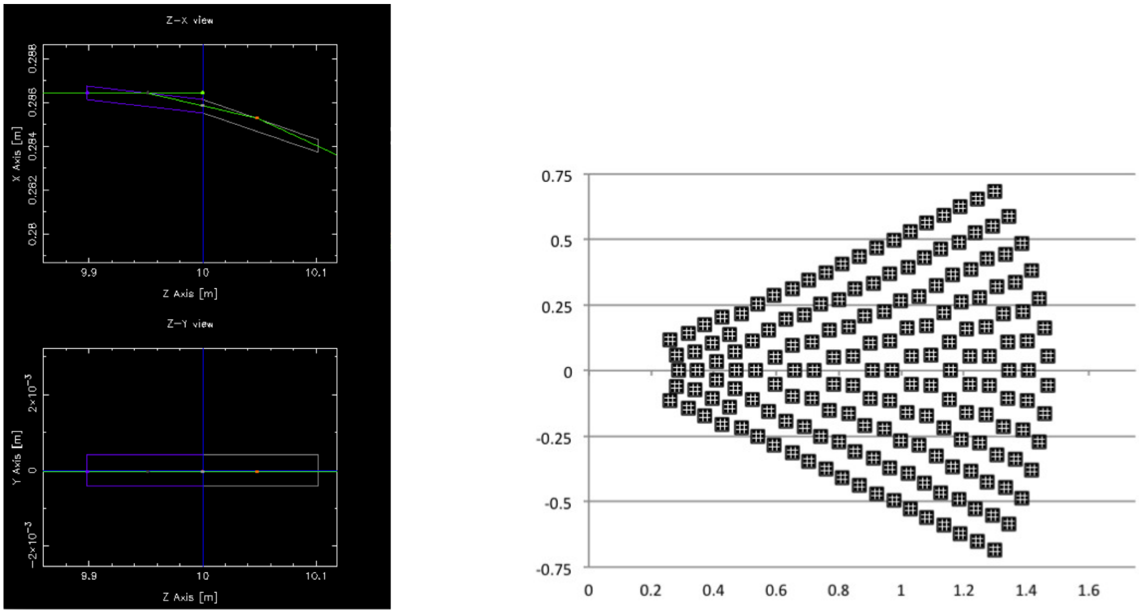

Figure 4. Left: A SPO pore set in McXtrace. Here we observe the pore geometry along the Z-axis. The parabolic (purple) and hyperbolic (grey) pores are seen along with the double reflection of a traced photon. Right: Graphic representation of the mirror modules positions considered for simulation.

4. SIMULATION OF PERFORMANCE

Flexibility of the code is crucial as several aspects of the geometry are still under investigation.[12] The variables considered as input parameters are: pore width and height (so far assumed to be 0.830 mm and 0.605 mm, figure 3), rib width (0.17 mm), rib pitch (1.0 mm), silicon wafer thickness (0.775 mm), membrane thickness (0.17 mm), SPO plate width (table 1), SPO length (table 1), height of mirror modules (number of stacked plates: 68 reflecting plates), number of mirror modules per row (table 2) position of mirror module within the optics, mid radius of mirror modules (table 1), parabolic radius and hyperbolic radius for each set of SPOs (table 1), telescopes focal length (12 m), Ir/B_4C bilayer coating throughout the whole optic and average surface roughness of the coating (assumed to be 0.45 nm).[16, 17, 25]

Using the latest available documentation on ATHENA as input,[14] we have simulated X-rays travelling through one set of pores (parabolic and hyperbolic) for each mirror module within one petal. That means that for each of the 177 mirror modules we ray traced the very central pore of the module. That means that we ray traced one pore per mirror module and assumed that the results for that one central pore is representative of the performance of the given mirror module. The performance of the pore within the mirror module is simulated individually based on its geometry and position. The results of pores are then combined to obtain the total telescope performance.

Figure 4 shows a SPO pore set in McXtrace. Here we observe the pore geometry along the Z-axis (focal axis). An example of parabolic (purple) and hyperbolic (grey) pores is seen along with the double reflection of a traced photon. The representation of the position of each mirror module considered for simulation is also seen.

For simulation of performance, we assume a perfect mirror and the effects of mirror deformations, displacement and misalignments have not yet been accounted for.

5. PRELIMINARY RESULTS

We evaluate the performance of the pores by ray tracing at two standard energies, 1 keV and 5 keV. Preliminary results include simulated on-axis effective area and performance per mirror module within the petal considered. To investigate the performance of the telescope for off-axis sources, we simulate photons arriving at the optics at a 10 arcmin off-axis angle and obtain the 10 arcmin off-area at 1 keV.

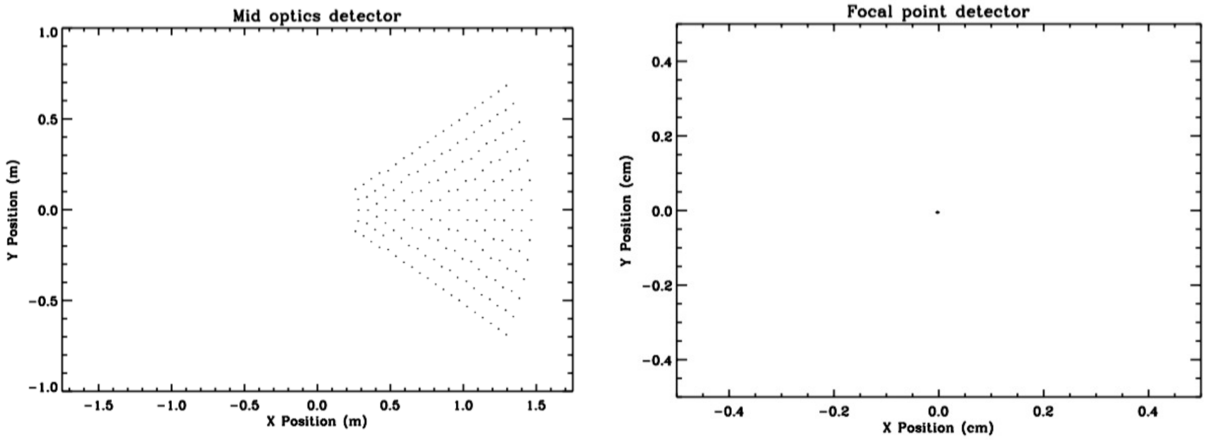

Figure 5. Left: Output from detector placed after the parabolic pores and before the hyperbolic pores registering all photons successfully reflected by the parabolic pores. Here is it possible to identity the petal structure and clearly see each central mirror module pore. Right: Detector placed at the focal point registering all photons successfully focused. Notice that the data from the focal point has been zoomed in with respect to the other data (left) by a factor 400 in each direction.

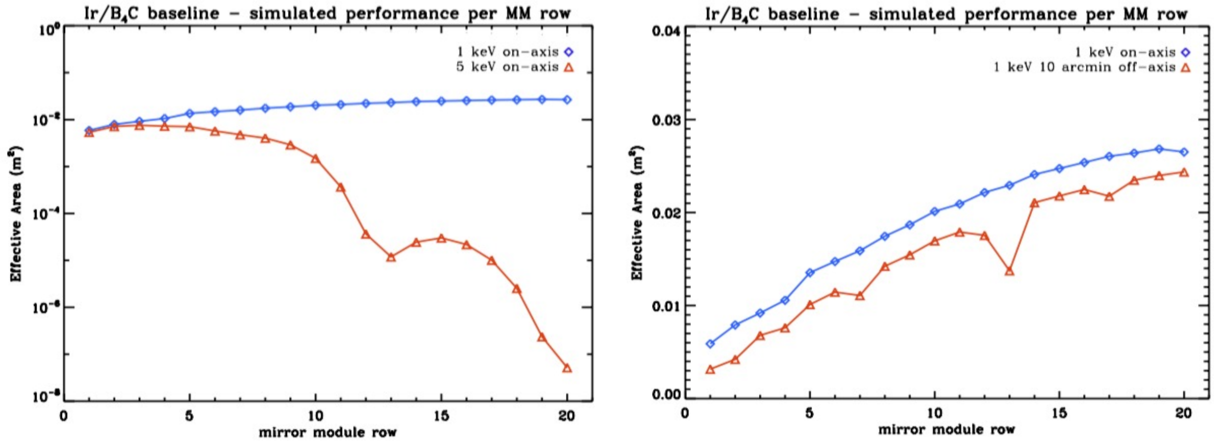

Figure 6. Left: Simulated on-axis effective area per mirror module row for 1 keV and 5 keV. Right: Contribution of each mirror module row to the on-axis effective area and 10’ off-axis effective areas at 1 keV.

Figure 5 the output from a detector placed after the parabolic pores and before the hyperbolic pores registering all photons reflected by the parabolic pores. The petal structure and the central mirror module pore are visible. The detector placed at the focal point registers all photons successfully focused, that means all photons reflected by both the parabolic and hyperbolic mirrors. As expected from a perfect geometry, all successful photons arrive exactly at the focal point.

Figure 6 shows the simulated on-axis effective area per mirror module row at 1 keV and 5 keV and the contribution of each mirror module row to the on-axis effective area and 10’ off-axis effective areas at 1 keV. The coating reflectivities generated using the software IMD considering the incident grazing angles at the centre of the mirror module rows are seen in figure 7. The theoretical model of the on-axis effective area along with the simulated effective areas (red) at 1 keV and 5 keV are also seen. We compare the simulated on-axis effective areas at 1 keV and 5 keV and find them to be in agreement with the theoretical model computed using the software IMD for the same pore geometry and mirror coatings.

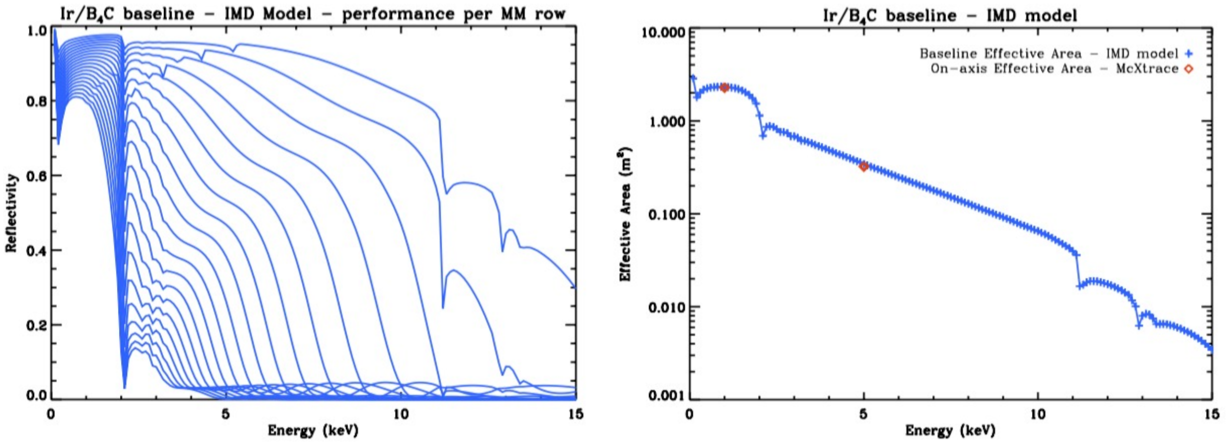

Figure 7. Left: Coating reflectivity theoretical model generated using IMD considering the incident grazing angles at the centre of the mirror module rows. Right: On-axis effective area theoretical model along with the simulated effective areas (red) at 1 keV and 5 keV.

6. SUMMARY AND DISCUSSION

We use the ray-tracing system McXtrace to simulate ATHENA's mirror performance and can successfully reproduce the focussing capability of the telescope geometry and coating performance (figures 5 - 7). At the present we have a working set of models on a pore level for the true Wolter-I ATHENA optic. We have tested the models for arbitrary position of pores/modules, specified as an input file and for the present baseline coating designs.

The output of the ray-tracings performed match well the on-axis theoretical models and seem to be a very accurate simulation of the expected geometry of the telescope. The simulation models allow for reflection on all four walls of a pore, at the present time we have considered reflections only on the coated surface. The pore-level models are currently not able to provide information on cross talk between pores and the possibility of implementation of cross talk on mirror model level will be evaluated.

As the design of ATHENA's optics is still under optimisation, the ray tracing tool is being developed to allow for flexibility in terms of geometry of the optics and the many listed input variables to the code.

Throughout this preliminary study we have assumed the surface roughness of the coated mirrors to be 0.45 nm and other values will be considered taking into consideration the latest experimental results available. Effects of surface roughness are being investigated by assuming reflectivity tables produced using the IMD software. The impact of coating design and coating uniformity will also be accounted.

No mirror deformations are considered in this study. In order to predict a realistic mirror performance, we expect in the next months to be able to implement scatter model and effects of mirror deformations, displacement and misalignments.

The use of McXtrace to simulate X-ray telescopes allows for the in-depth analysis of in-orbit performance and for laboratory X-ray test results.

ACKNOWLEDGMENTS

The simulation of ATHENA's optics using McXtrace is part of the SIMPOSium project, which includes investigation of several physical processes such as geometry design, stray light simulations, diffractive effects among other processes affecting the performance of ATHENA.

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