ATHENA optimized coating design

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ABSTRACT

The optimization of coating design for the ATHENA mission is described and the possibility of increasing the telescope effective area in the range between 0.1 and 10 keV is investigated. An independent computation of the on-axis effective area based on the mirror design of ATHENA is performed in order to review the current coating baseline. The performance of several material combinations, considering a simple bi-layer, simple multilayer and linear graded multilayer coatings are tested and simulation of the mirror performance considering both the optimized coating design and the coating baseline including on- and off-axis effective area curves are presented. We find that the use of linear graded multilayers can increase the effective area of ATHENA in the energy range between 0.1 keV and 15 keV.

Keywords: X-rays, ATHENA mission, Coating optimization, Multilayers, Ray-tracing

1. INTRODUCTION

The optimization of the mirror coatings for the ATHENA Mission is aimed at increasing the on- and off-axis effective area in the energy range between 0.1 keV and 10 keV. The reference effective areas for ATHENA are 1.15 m^2 at 1.25 keV and 0.5 m^2 at 6 keV. There are no specifications at higher energies.

The basis of the optimization is the use of a heavy (absorber) reflecting layer combined with a light (spacer) material on top to boost reflection at the low energy range up to 5 keV and the use of multilayer coatings to maximize throughput at the intermediate energy range between 5 keV and 10 keV.

X-ray reflection from layered structures is determined by the optical constants comprised of the refractive index n and the extinction coefficient k of the constituent materials. n and k vary with energy and the reflectance of an interface is directly related to the optical contrast between its two materials. However, the overall reflectance from several interfaces is further limited by the extinction coefficient of the materials. Therefore, the optimum material combinations are those that combine relatively large difference between n and k, while keeping the extinction coefficient low. The study of material combination starts by selecting spacer candidates with minimum absorption followed by the choice of absorber candidates with maximum contrast. It is also necessary to take into account the physical and chemical compatibility of the materials.

The graze angle range for ATHENA is 3.26 mrad to 19.57 mrad, assuming an inner radius of 0.15 m and an outer radius of 0.9 m. Different types of coatings can be considered for different graze angle ranges. In this study, the optimum materials combinations favoring a low energy range and a intermediate range are considered.

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1.1 The low energy range

Previous X-ray observatories have largely relied on the use of simple metal coatings to achieve a high throughput for energies up to 10 keV. This is based on maximizing the critical angle for total external reflection and thus achieve maximum overall throughput.

It has been demonstrated recently that the use of an overcoat of a light material can enhance the throughput at energies between 0.5 and 5 keV without jeopardizing the throughput at higher energies.[1] This is due to the fact that below the critical angle the reflectance of a light material is higher than that of a heavy material due to a smaller extinction coefficient, which also allows for the higher energies to penetrate to the heavy material and be reflected from this without considerable loss. A coating optimization is based on optimizing a figure of merit defined by the choice of materials and the thickness of each material. Candidates for the light material are Si, Al, C, B and compounds like SiC and B_4C, candidates for the heavy material are W, Re, Pt, Ni and Ir.

It has been found that a layer of Ir with a C overcoat provides a good overall enhancement.[1] However, issues in the Silicon Pore Optics stacking process make the use of C questionable. It was necessary to find another light material to work as a replacement for C and B_4C is the only material from the list above promising similar results.

Ir coatings are highly stressed but investigations on how to reduce the coating stress to a satisfactorily level are being carried out at DTU Space. A method under investigation is to apply an initial layer of Cr, which has opposite stress and thus can balance the overall stress[2,3] . A Cr undercoat could lead to higher roughness of the Ir/B_4C interfaces.[3] An option is to replace Ir by either W or Pt, which may not require the use of an undercoat.

An alternative approach to obtain the required effective area in the low energy range and at the same time increase the area at higher energies is to use a linear graded multilayer. The use of a linear graded multilayer will only be beneficial in this case if a top bi-layer, similar to the one described above, is added on top of the multilayers; otherwise there will be losses in the throughput at low energies. The following material combinations are considered for multilayers:

W/Si: Known to form very stable smooth interfaces with low stress (stress $\approx$ -100MPa).

Pt/B_4C: Unknown properties at present, under investigation.

Ir/B_4C: Initial results indicate reasonably smooth interfaces. The coating is stressed (stress $\approx$ -2GPa) and may require a Cr undercoat which could jeopardize roughness.

W/B_4C: Known to be a high stress coating with smooth interfaces.

1.2 The mid energy range

To increase the throughput over that of the current baseline using just Ir with an B_4C overcoat in the energy range between 5 keV and 10 keV, the addition of a multilayer is necessary. This is particularly interesting for the outer radius range where an Ir/B_4C bi-layer coating no longer adds to the effective area beyond 6 keV. A multilayer coating will improve the throughput in the mid energy range.The material choices for the multilayer coating are listed in 1.1

2. BASELINE DESIGN

The baseline design chosen for the ATHENA mission consists of two identical telescopes with fixed focal planes, the first containing a calorimeter spectrometer and the second a wide field imager. For the results presented in this study we take an ESA reference design with telescope focal length of 11.5 m, telescope innermost radius of 0.15 n and outermost radius of 0.90m. The operational energy range is from 0.1 keV to 10 keV.

A conical approximation of Wolter-I design is adopted making use of Silicon Pore Optics (SPO) technology.[4] For each telescope, mirror modules of double-stacked mirror plates populate one petal. A petal consists of 12 rows of mirror modules, of which only the first seven rows form a complete circle, with the outer rows partially filled, making an owl-like design.

Each mirror module consists of two times two stacks of 35 mirror plates of which 34 are reflecting and one is obscured. That gives a total of two times 68 mirror plates contributing to the telescopes effective area per mirror module.

The length and width of the mirror plates depend on the radial position of the mirrors modules. The plates in the same mirror module have same dimensions. The plate dimensions vary depending on the row it belongs to. The mirror plates are wedged and ribbed, and have a pore size of 0.605 mm by 0.83 mm. The number of pores per plate depends on the plate width. The ribs have a width of 0.17 mm and a pitch of approximately 1 mm. Figure 1 illustrates the mirror plate concept.

The coating recipe adopted as baseline is a bi-layer: 8nm of B_4C layer on top of a 10nm Ir layer. The same coating is adopted for all mirror modules at all radii.

2.1 Analytical calculation of on-axis effective area

The on-axis effective area A_{eff} is defined as

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

In equation 1, A_p is the mirror plate pore area, $R(E,\alpha)$ is the mirror reflectance, and n_p is the total number of pores for all reflecting mirror plates.[5]

Following a conical approximation, the incident grazing angle α is given by

$$\tan 4\alpha = \frac{r}{F_L} \quad , \tag{2}$$

where F_L is the focal length (11.5 m) and r the radius.

The mirror reflectance is dependent on the energy and incident grazing angle α. To compute the mirror reflectance we use the IDL software package IMD,[6] considering the energy range between 0.1 keV and 10 keV, and grazing angles corresponding to radii between 0.15 m and 0.90 m.

$$A_p = D_p \cdot W_p \quad . \tag{3}$$

For each row of mirror modules the number of pores n_p per mirror plate is different, varying according to the plate width,

$$n_p \cdot (0.17 + W_p) + 0.17 \cong P_w \quad . \tag{4}$$

The number of pores per plate for each row is listed in table 1.

2.2 Review of ATHENA baseline design

The effective area calculated based on the coating baseline, with a 10 nm Ir layer with a 8 nm B_4C layer on top, is presented in table 2 and illustrated in figure 2. The computed effective areas were reduced by 10% in order to account for eventual losses, such as alignment losses and losses due to particulate contamination.

For the initial calculations, a perfectly smooth surface was considered, with surface roughness set to zero, but because a perfectly smooth surface is unrealistic, the effective area considering more sensible roughness values were also computed.

A surface roughness of about 3 Å is measured at the 8 keV facility at DTU Space for a pure Si substrate, measurements of wedged mirror plates yields an average surface roughness of 4.5 Å. The introduction of an Cr undercoat to reduce coating stress increases the surface roughness to 6.5 Å.[3]

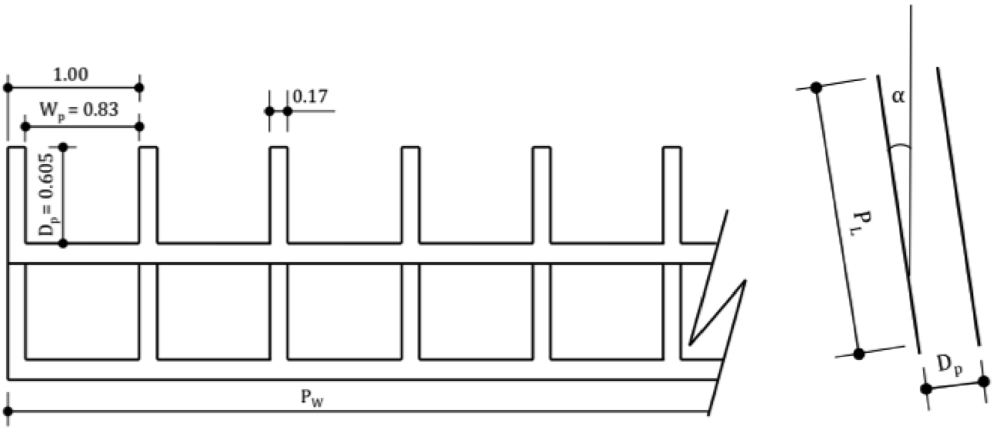

Figure 1. (Left) Silicon Pore Optics geometry considered for computing the pore size, area and number of pores, values listed in mm, not to scale. (Right) Schematic of the mirror pore and grazing incident angle α. P_W is the plate width, P_L the plate length, D_p is the pore depth and W_p is the pore width.

Row	Mirror modules	Reflecting plates	Pores per plate	Middle Radius [m]
1	11	2 × 748	74	0.184
2	15	2 × 1020	75	0.246
3	18	2 × 1224	82	0.308
4	21	2 × 1428	86	0.370
5	25	2 × 1700	85	0.433
6	28	2 × 1904	88	0.495
7	31	2 × 2108	90	0.557
8	24	2 × 1632	89	0.619
9	22	2 × 1496	91	0.681
10	18	2 × 1224	90	0.744
11	18	2 × 1124	92	0.806
12	14	2 × 952	93	0.868

Table 1. Overview of mirror plates for ATHENA baseline design.

Energy	Required A_{eff} $\sigma = 0$	Reviewed A_{eff} $\sigma = 0$	Reviewed A_{eff} $\sigma = 3$	Reviewed A_{eff} $\sigma = 4.5$	Reviewed A_{eff} $\sigma = 6.5$
1.25 keV	1.15	1.172	1.167	1.161	1.148
6 keV	0.50	0.517	0.497	0.473	0.432

Table 2. Comparison between on-axis affective areas (A_{eff}) computed considering different values of surface roughness (σ). Roughness values are listed in Å and effective area in m^2.

The loss in effective area due to surface roughness is only marginal at low energies, the values computed considering surface roughnesses of 3 Å and 6.5 Å only differ by ≈ 1.5 % at 1.25 keV. At 6 keV the loss in effective area is more significant, and a reduction of 13% in effective area is observed comparing the computations assuming surface roughnesses of 3 Å and 6.5 Å. The effective areas computed considering different surface roughness are shown in figure 2 and listed in table 2. Possible approaches to reduce the surface roughness are currently being investigated at DTU Space.

Figure 2 presents the ATHENA reflectance as a function of radius computed at different energies considering the Ir/B_4C coating baseline. The coating baseline for ATHENA clearly favors the low energy range, between 0.1 keV and 2 keV. The reflectance curves for the Ir/B_4C bi-layer baseline shows excellent reflectance at 1 keV and 2 keV, while the intermediate energy range, 6 keV and 10 keV, higher reflectance values can be achieved by adopting a multilayer coating. Including a multilayer coating underneath the bi-layer coating would increase the effective area at the intermediate energy range without compromising the low energy range.

We also bear in mind that the baseline detector for the Wide Field Imager has an energy range up to 15 keV, and it is desirable to consider the possibility of improving the effective area in the 10 keV to 15 keV band.

3. COATING OPTIMIZATION

3.1 Material selection - Bi-layers

The choice of coating recipes is based on optimization over different energy ranges. The use of a simple bi-layer coating is appropriate for energies lower than 5 keV, while to improve the telescope performance above 5 keV the use of multilayers is required.

The criterion applied for the choice of a simple bi-layer coating material is based on the integrated on-axis effective area over the energy range between 0.1 and 15 keV. The telescope is divided in 12 regions corresponding to the 12 mirror module rows defined by the ATHENA design. We computed the best coating thickness for each material combination in order to maximize the integrated on-axis effective area. The surface roughness considered is 6.5 Å for Ir/B_4C, and 4.5 Å for W/Si, W/B_4C and Pt/B_4C. Under this criterion, we find that both the current ATHENA baseline (10 nm Ir, 8 nm B_4C) and the optimized Pt/B_4C bi-layer (11 nm Pt, 11 nm B_4C) return the best overall results and are therefore the prefered bi-layer choices.

3.2 Material selection - Multilayers

To enhance the telescope effective area over the energy range 5 - 10 keV, a multilayer coating approach is suggested. Also here the material choice is defined by evaluating the integrated on-axis effective area over the energy range between 0.1 and 15 keV. A simple multilayer coating is considered for the materials listed in 3.1 with a cap layer of the heaviest material in the multilayer and an 8 nm overcoat of B_4C to account for the energies below 1.5 keV. The surface roughness applied is 6.5 Å for Ir/B_4C and 4.5 Å for the remaining material combinations.

The parameters considered in the computation are: number of bi-layers, thickness of the bi-layers, ratio between heavy and light material thickness (Γ), and thickness of the cap layer of the heavy material. The best parameters for each material choice return maximum integrated on-axis effective area.

Applying a multilayer of Pt/B_4C results in the best performance considering the criterion above while W/Si, W/B_4C and Ir/B_4C demonstrate equivalent performances. The material combinations W/Si, W/B_4C and Ir/B_4C return integrated on-axis effective areas that differ from the computed for Pt/B_4C by only 2.5%. There are several reasons for choosing Pt over W, e.g. the absorption edges around 1-2 keV.

Stress and increased surface roughness indicates that Ir/B_4C coatings may return poor performance as multilayers. The selected materials for multilayer coating optimization are Pt/B_4C, W/Si and W/B_4C.

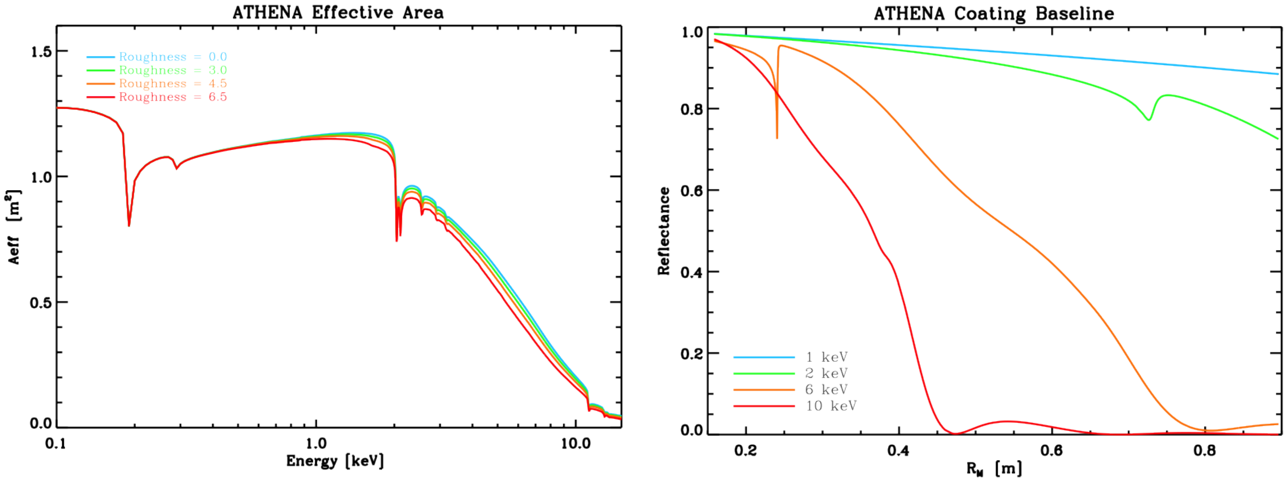

Figure 2. Left: ATHENA effective area as a function of energy. The effective areas computed considering different surface roughness are indicated. The losses due to roughness are particularly significant at higher energies. Right: ATHENA reflectance as a function of radius R_M for different energy values considering the Ir/B_4C coating baseline and assuming a surface roughness of 6.5 Å.

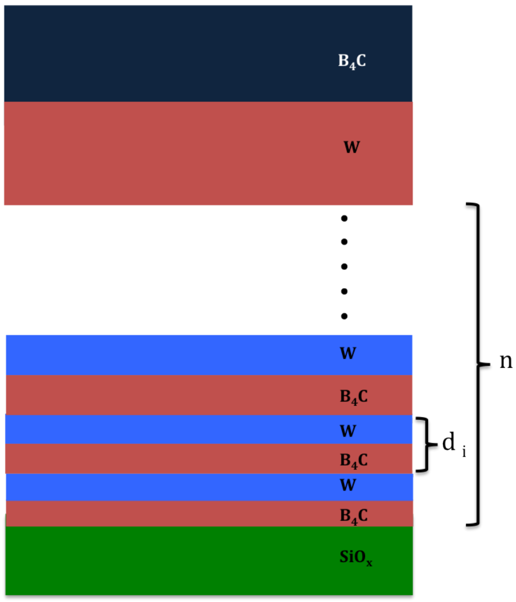

Figure 3. Schematic of coating configuration.

4. THE OPTIMIZED DESIGN

4.1 Analytical approach

To optimize the coating design using multilayers we considered 12 different coating recipes, one for each mirror module row. The motivation for this choice is to investigate the possibility of a better performance over the bi-layer coating for all rows and the need of a smooth effective area curve at the scientifically interesting energy region around 6 keV.

To optimize a wider energy range a linear graded multilayer is chosen over a simple multilayer. The optimized material combinations are: a linear graded Pt/B_4C multilayer with a Pt cap layer on top of the multilayer and an 8 nm B_4C overcoat, a linear graded W/Si multilayer with a W cap layer and an 8 nm B_4C overcoat, and a linear graded W/B_4C multilayer with a W cap layer and an 8 nm B_4C overcoat. The B_4C overcoat is optimized for best performance at 1 keV and is therefore 8 nm. A schematic of coating configuration is shown in 3.

For each mirror module row an optimal coating recipe is computed in order to maximize the on-axis effective area in the region around 6 keV without compromising the effective area at lower energies. This is achieved by evaluating the several possible parameter combinations that result in the maximum integrated effective area over energy for the energy range between 0.1 keV and 10 keV with the condition that the loss of effective area between 1 and 5 keV is minimal.

To avoid solutions that maximize the integrated on-axis effective area but are not smooth between 4 keV and 6 keV, a figure of merit is defined so that the integrated effective area is multiplied by a Gaussian function with peak at 5 keV.

$$F.O.M = \int_{0.1}^{10} A_{eff}(E) \cdot ae^{-\frac{(E-b)^2}{2c^2}} dE \quad . \tag{5}$$

In equation 1, A_{eff} represents the on-axis effective area, E is the energy, the parameters of the Gaussian function are a = 1.0, b = 5.0 and c = 1.5, and the integration is computed from 0.1 to 10 keV.

The parameters considered in this computation are: number of bi-layers (n), thickness ratio between heavy and light material (Γ), minimum bi-layer thickness (d_{min}), maximum bi layer thickness (d_{max}) and thickness of the cap layer (d_c) (to accommodate the energies between 1.5 keV and 5 keV). The parameters were varied considering steps of five bi-layers, 0.1 for Γ, 5 Å for d_{min} and d_{max} and 5 Å for d_c. Figure 3 illustrates the coating configuration for W/B_4C multilayer.

For all mirror module rows we find that the multilayer coatings perform better in the energy range between 5 and 10 keV. The best coating parameters are listed in tables 3 - 5. The optimized effective areas over energy are shown in figure 4.

The computed on-axis effective areas for both the Ir/B_4C baseline and the optimized multilayer coatings at 1 keV, 4 keV, 6 keV and 8 keV are listed in table 6. The surface roughness applied are 6.5 Å for the baseline and 4.5 Å for the optimized multilayers. The improvement in the on-axis effective area at 6 keV compared to the baseline performance is listed in table 7. The on-axis effective area curve for the baseline and optimized recipes are shown in figure 4.

5. SIMULATION OF MIRROR PERFORMANCE

To simulate ATHENA mirror performance we make use of the ray-tracing system for X-ray telescopes MT RAYOR,[7] developed at DTU Space and already applied other X-ray missions such as NuSTAR.[8]

The telescope geometry was set to closely match the actual ATHENA design. Both plate ribs and obscuration between the mirror modules rows were introduced. Figure 5 shows ATHENA aperture considered for ray tracing.

The simulated mirror performance considering the baseline design and the W/Si optimized multilayer, on- and off-axis are shown in figure 6.

For the ray tracing, a perfect mirror was assumed with the inclusion of an energy independent scattering component that leads to a half energy width of 10". A 10% loss in the effective area is considered to account for eventual losses due to e.g. mirror deformations, alignment and particle contamination.

Row	N	Γ	d_{min} [nm]	d_{max} [nm]	d_W [nm]	A_{I+}[%]
1	5	0.6	5.0	21.0	12.0	1.15
2	5	0.6	5.0	20.5	12.0	-0.08
3	5	0.6	5.0	17.5	12.0	-0.44
4	5	0.6	5.0	15.5	12.0	0.67
5	5	0.6	5.0	12.5	12.0	1.74
6	5	0.6	5.0	11.0	11.0	2.67
7	10	0.6	3.0	10.5	9.0	3.25
8	10	0.6	3.0	10.0	8.0	2.76
9	10	0.6	4.0	9.5	7.0	2.09
10	10	0.6	5.0	9.0	6.0	0.37
11	10	0.6	4.5	8.5	6.0	0.33
12	10	0.6	4.5	8.0	6.0	-0.91

Table 3. Optimized coating design for ATHENA assuming a linear graded W/Si multilayer. A_I represents the improvement in integrated effective area over the baseline in the energy range between 0.1 and 15 keV.

Row	N	Γ	d_{min} [nm]	d_{max} [nm]	d_W [nm]	A_{I+}[%]
1	5	0.6	5.0	21.0	12.0	2.79
2	5	0.6	5.0	19.5	12.0	4.23
3	5	0.6	5.0	17.5	12.0	4.54
4	5	0.6	5.0	15.5	12.0	4.04
5	5	0.6	4.0	12.5	12.0	3.42
6	5	0.6	5.0	11.0	11.0	3.68
7	5	0.6	5.0	10.0	9.0	4.31
8	5	0.6	5.5	9.5	8.0	3.57
9	10	0.6	4.0	9.0	7.0	3.23
10	10	0.6	4.5	8.5	6.0	1.94
11	10	0.6	3.0	8.0	6.0	2.11
12	10	0.6	4.0	8.0	6.0	1.55

Table 4. Optimized coating design for ATHENA assuming a linear graded Pt/B_4C multilayer. AI represents the improvement of integrated effective area over the baseline in the energy range between 0.1 and 15 keV.

Row	N	Γ	d_{min} [nm]	d_{max} [nm]	d_W [nm]	A_{I+}[%]
1	5	0.6	5.0	21.0	12.0	0.96
2	5	0.6	5.0	20.5	12.0	-0.39
3	5	0.6	5.0	17.5	12.0	-0.83
4	5	0.6	5.0	15.5	12.0	0.39
5	5	0.6	5.0	12.5	12.0	1.46
6	5	0.6	5.0	11.0	11.0	2.49
7	10	0.6	3.0	10.5	9.0	3.18
8	10	0.6	3.0	10.0	8.0	3.27
9	10	0.6	4.0	9.5	7.0	2.90
10	10	0.6	5.0	9.0	6.0	1.70
11	10	0.6	4.5	8.5	6.0	1.48
12	10	0.6	4.5	8.0	6.0	0.78

Table 5. Optimized coating recipe for W/B_4C.

	Baseline Ir/B_4C bi-layer	Optimized Pt/B_4C bi-layer	Optimized W/Si, ML	Optimized Pt/B_4C, ML	Optimized W/B_4C, ML
A_{eff} at 1keV	1.145	1.160	1.153	1.149	1.153
A_{eff} at 4keV	0.676	0.673	0.673	0.663	0.672
A_{eff} at 6keV	0.429	0.446	0.482	0.488	0.491
A_{eff} at 8keV	0.260	0.273	0.269	0.282	0.272

Table 6. Comparison between baseline and optimized coating performances. On-axis effective areas computed assuming surface roughness of 6.5 Åfor the Ir/B_4C baseline and 4.5 Å for the optimized coating recipes.

Optimized Pt/B_4C bi-layer	Optimized W/Si, ML	Optimized Pt/B_4C, ML	Optimized W/B_4C, ML
3.96	12.35	13.75	14.45

Table 7. Effective area improvement [%] over baseline at 6 keV, computed assuming surface roughness of 6.5 Å for the Ir/B_4C baseline and 4.5 Å for the optimized coating recipes.

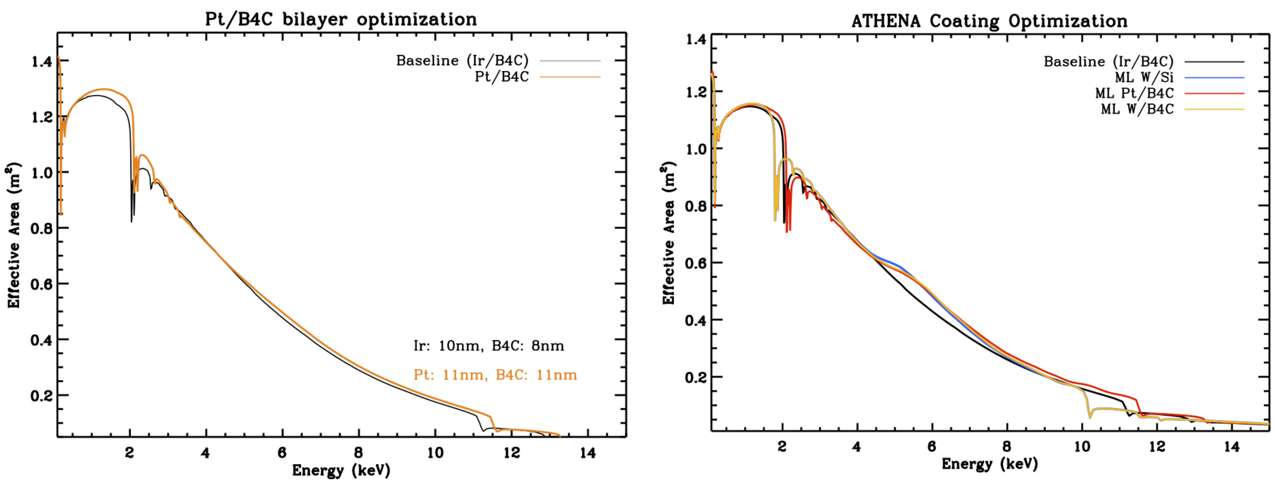

Figure 4. Coating optimization. Left: Baseline and optimized Pt/B_4C bilayer. Right: Baseline and optimized multilayers.

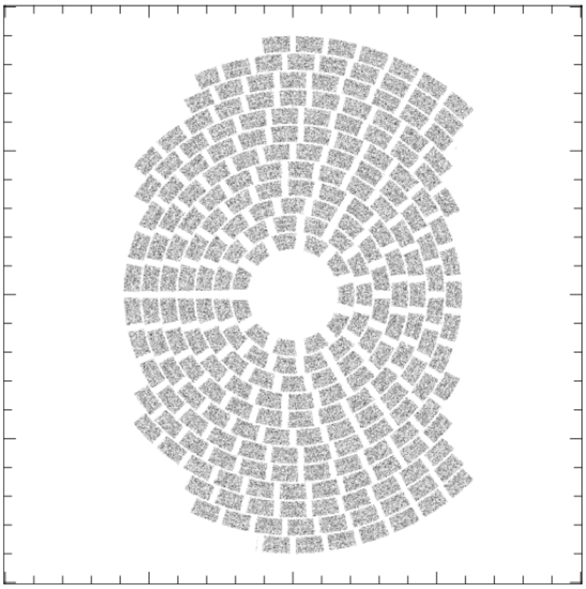

Figure 5. ATHENA aperture considered for simulation of mirror performance through ray tracing.

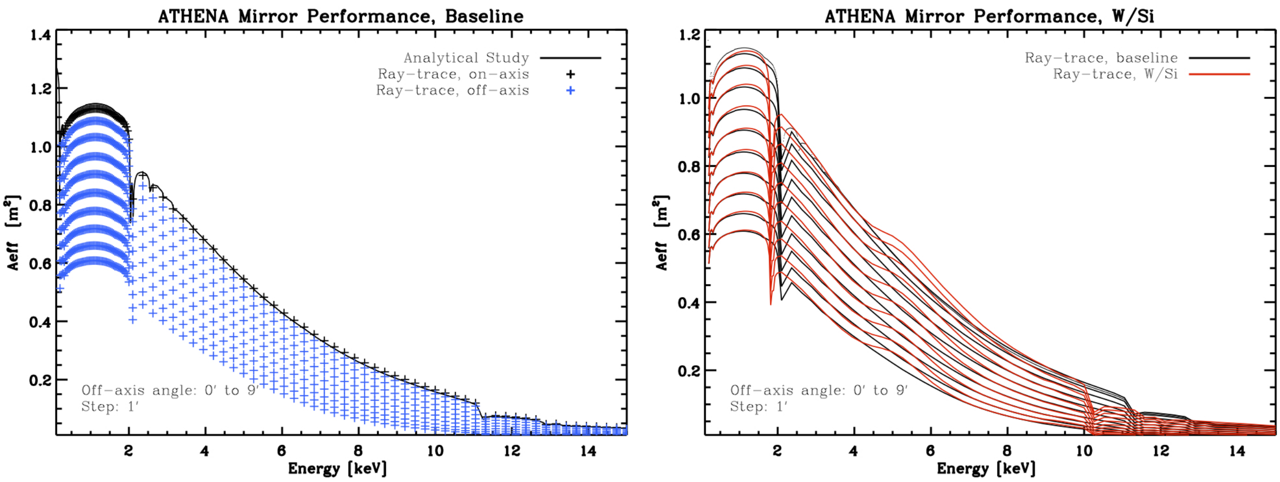

Figure 6. Left: Simulated mirror performance considering ATHENA coating baseline. Right: Simulated mirror performance considering ATHENA optimized W/Si coating design. Results presented considering two telescopes, 10% reduction applied. The off-axis angle varies between 0 and 9”, with a step of 1”.

6. SUMMARY

We investigated the possibility of increasing the effective area of the ATHENA mission by means of optimizing the mirror coatings. A review of the current coating baseline design shows the effect of surface roughness on the performance of the coatings. The effective area computed at 6 keV assuming a surface roughness of 6.5 Å is 13% lower than the effective area obtained for roughness of 3.0 Å, showing the increasing effect of the roughness at intermediate energies. The need of a Cr undercoat to reduce stress in the Ir/B_4C coating causes an increase in the surface roughness. We find that a bi-layer of Pt/B_4C can work as an alternative to the current coating baseline with equivalent performance.

The use of linear graded multilayer underneath the bi-layer coating has proven to increase the telescope effective area over the energy range between 5 keV and 10 keV without losses in the low energy range. Comparing the performances of the current coating baseline and the optimized linear graded multilayers, we observe an increase of 12.35% in effective area at 6 keV when considering a W/Si multilayer, 13.75% for a Pt/B_4C multilayer, and 14.45% increase for W/B_4C multilayer, making it clear that improvement over the current coating baseline design can be achieved.

To simulate the performance of the mirror coatings, a ray-tracing system was set to closely match the ATHENA geometry. By simulating the mirror performance, the on- and off-axis effective areas considering both the coating baseline and an optimized coating design are assessed.

Combined experimental and theoretical studies for further optimizing the coatings for ATHENA are under investigation at DTU Space and will be reported in the near future.

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