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Enhanced Simulations on the Athena/Wide Field Imager instrumental background

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ABSTRACT

The Wide Field Imager (WFI) is one of two focal plane instruments of the Advanced Telescope for High-Energy Astrophysics (Athena), ESA's next large X-ray observatory, planned for launch in the early 2030's. The current baseline halo orbit is around L2, the first Lagrangian point of the Sun-Earth system, L1 is under consideration. For both potential halo orbits the radiation environment, solar and cosmic protons, electrons and He-ions will affect the performance of the instruments. A further critical contribution to the instrument background arises from the unfocused cosmic hard X-ray background. It is important to understand and estimate the expected instrumental background and to investigate measures, like design modifications or analysis methods, which could improve the expected background level in order to achieve the challenging scientific requirement ($< 5 \times 10^{-3}$ cts/cm²/keV/s at 2 - 7 keV). Previous WFI background simulations¹ done in Geant4 have been improved by taking into account new information about the proton flux at L2. In addition, the simulation model of the WFI instrument and its surroundings employed in GEANT4 simulations has been refined to follow the technological development of the WFI camera.

Keywords: Athena/WFI, Instrumental Background, Space Environment, Particle Environment, GEANT4
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1. INTRODUCTION

1.1 Description of Wide Field Imager (WFI) Instrument

A comprehensive description of the WFI instrument is provided in Ref. 2. Here we give a short summary of the main relevant components. This work is an update of Ref. 1 and hence contains similar descriptions of the WFI, key-Science drivers, background components and GEANT4/GRAS. The WFI will provide important scientific capabilities to the mission. The Large Detector Array (LDA) will offer an unprecedented survey capability with its 40'×40' field of view properly sampling the point spread function (5" HEW on-axis) provided by the Athena mirror system.

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This is achieved by employing a large area, almost $14 \times 14 \text{ cm}^2$ sized, silicon based detector in the focal plane.

The signal electrons, generated by an incoming X-ray photon are collected and amplified in active pixels sensors of DEPFET (depleted p-channel field effect transistors) type, which are integrated onto a back-illuminated fully depleted $450 \mu\text{m}$ thick silicon bulk. They are providing state-of-the-art energy resolution in the full energy range (0.2 to 15 keV). The pixel size of $130 \mu\text{m} \times 130 \mu\text{m}$ is well matched to the performance of the mirror system. The measurement of the arrival time of the X-ray photon is determined by the anticipated read-out time of 5 ms. Since the required size of the large detector cannot be realized with the diameter of available ultra-pure Si wafers, it is subdivided into four quadrants with $67 \times 67 \text{ mm}^2$ each, leading to insensitive gaps between the quadrants. A work-around for this deficiency are dithering observations of the sky-region of interest. In total 1024×1024 DEPFET pixels are placed on the full detector plane, resulting in 512×512 pixels per quadrant. Each quadrant is controlled independently by 8 Switcher-A ASICs and read out by eight Veritas-2 ASICs (for details of the electronic concept see Ref. 2). In order to derive a lower power consumption the DEPFETs are operated in rolling shutter mode, which means: one DEPFET line is switched on while the others accumulate photons without power consumption. Both sides of the Si-sensor exhibit coatings, a $5 \mu\text{m}$ BCB (Benzocyclobutene) thick layer on the off-mirror side serves for passivation and a 90 nm thick aluminum coating on the mirror side of the detector serves as on-chip filter to reduce the contamination of the X-ray signal by optical light.

The large area imaging capability of WFI is complemented by the addition of a smaller $8.3 \times 8.3 \text{ mm}^2$ sized fast timing detector, employing the same DEPFET technology. The so called Fast Detector (FD) is placed aside the large detector and is defocused by about 35 mm in order to allow for a high throughput during observations of bright sources of about 1 Crab intensity. The FD with 64×64 pixels is controlled and read out in two halves in parallel, thus improving the time resolution by a factor of two, allowing to fulfill the high time resolution requirement of $80 \mu\text{s}$.

The LDA and FD, together with control and analogue frontend electronics (AFE, CFE) are surrounded by an aluminum shield, which is intended to reduce the proton flux to the detector in order to mitigate the radiation damage. With the planned thickness of 3 cm Al equivalent the shield is able to stop, on average, protons up to $\sim 110 \text{ MeV}$.

As outcome of the presented and previous studies (Ref. 1) a graded-Z shield will be mounted as an extra layer inside the proton shield in order to suppress Al-fluorescence radiation at $\sim 1.5 \text{ keV}$. In addition it will reduce the contribution of secondary photons from primary proton interactions and Compton scattered primary hard X-rays. Much work has been done in the past to optimise the graded z-shield in order to minimize the instrumental background due to secondary and primary electrons and photons (Ref. 1). Bringing together past and current background studies and a feasibility analysis the current baseline for the graded z-shield is 3 mm of Molybdenum and on top $40.6 \mu\text{m}$ of Polyimide (Kapton), with the Polyimide facing towards the detector. The Polyimide will most probably be glued to the Molybdenum using an epoxy adhesive. This adhesive needs to be taken into account in background simulations as it will contribute to the suppression of fluorescence lines.

In addition to the above described camera head, consisting of Si-detector, proton shield and graded-Z shield the WFI instrument has a filter wheel (FW) in front of the camera as well as an optical stray-light baffle (see Fig. 4). The filter wheel allows to move four different slots in front of the LDA, a UV and visible light blocking filter, an open position for efficient evacuation of the filter wheel and camera head, a closed position for sensor protection and instrumental background measurements, and a position that hosts the on-board calibration sources.

1.2 Key Science Drivers for Requirements on Athena Background

Key science objectives for the WFI have been identified within the framework of Athena's "Hot and Energetic Universe" science theme.³ These objectives (see also Ref. 4), include, e.g., the search for the active galactic nuclei at redshifts 6–8, which will appear as very faint point sources in the anticipated multi-tiered WFI survey.⁵ The same survey will also push the surface brightness sensitivity to detect the extended emission of the first galaxy groups, i.e. the first building blocks of the dark matter structure filled with hot gas at redshifts around 2.⁶ In the nearby Universe, WFI observations of the very low surface brightness regions in the outskirts of galaxy clusters will allow the determination of the physical processes dominating the injection of non-gravitational energy into

the intra-cluster medium as well as its chemical abundances.⁷ Achieving those and many more science objectives will rely fundamentally on a low and well characterized background.

The WFI background requirement on the background intensity is divided between X-ray sky components, which dominate the background spectrum below ~ 2 keV, and particle components that emerge above. Most of the work done thus far within the WFI Background Group has concentrated on the latter, not because the former are of little consequence but because at this time it is important to concentrate efforts on particle components. The background requirements are driven by the WFI science goals. Generally speaking X-ray sky requirements, such as those on the stray X-ray light, are critical to achieve much of the survey goals while requirements on particle components, are of great relevance for the characterization of cluster outskirts.

According to ESA's Athena Science Requirements Document ent (SRE-S/ATH/2020/02) the requirement on the intensity of the quiescent particle background is:

- "Athena shall achieve a (focused and not focused) non-X-ray background for wide-field observations of $< 5.5 \times 10^{-3}$ cts/cm²/keV/s between 2–7 keV. The contribution by the non-focused component corresponds to a reference model and flux of the Galactic Cosmic ray component, defined as follows: 80% of the flux of the GCR model during solar minimum as described in Equations (1) and (2) with $\phi = 379.3$ MV, as presented in the document "Consolidation of the absolute level of the Galactic Cosmic Ray (GCR) protons spectrum"⁸ and forthcoming Ref. 9." This should ensure that for e.g. faint clusters or outskirts of clusters with low surface brightness spectral features at 6 keV or the Bremsstrahlung exponential cut-off can be determined.

The non-X-ray background refers to events not registered as cosmic X-ray events (direct particles and secondaries), which fall in the X-ray band between 0.2 and 15 keV. The spectra of incoming particles (at solar minimum) and unfocused photons are given in Fig. 1. For the presented studies 80% of the solar minimum and therefore cosmic ray maximum flux is used.

Figure 1. (a) The spectra of cosmic protons,⁸ electrons¹⁰ and He-ions.¹¹ (b) The spectrum of diffuse cosmic hard X-rays measured with HEAO-1.¹²

2. BACKGROUND COMPONENTS

2.1 The Charged Particle Background

In the following we briefly discuss the components of the charged particle background, which depend only mildly on the final orbit of the satellite. The current baseline orbit for Athena is around the second Lagrangian Point (L2) of the Sun-Earth system.

The charged particle environment of both L1 and L2 comprises:

- **GCR** Galactic Cosmic Rays (GCR) include protons, electrons, and He ions with energies from several tens of MeV to several GeV. At the considered orbits, the GCR are subject to variations over the solar cycle. Here, low energetic particles vary more than high energetic ones, i.e. 200 MeV protons vary by more than a factor of two between Solar maximum and minimum, while at 2 GeV this variation is only 10%. The studies presented in this document use an updated spectrum for the galactic protons. This spectrum has been derived to give the most conservative estimate of the GCR proton spectrum and is based on data from Voyager2, SOHO and PAMELA satellites and neutron monitor (NM) measurements Ref. 9. Spectra of GCR protons, electrons and He ions are shown in the left panel of Fig. 1.
 - **SEP** Solar Energetic Particles (SEP) are mostly protons of accelerated by the Sun to up to 10-100 MeV. They are characterized by increases in the particle flux of several orders of magnitude.
 - **STI** Supra-Thermal Ions (STI) are mostly protons accelerated in the Heliosphere to energies extending up to several hundred keV. They vary significantly on time scales from a few seconds to hundreds of ks, potentially correlated with the Solar cycle. At L2, an additional STI component from the Earth's magneto-tail is expected.
- SEP and STI contribute to the concentrated particle background component. These are mostly protons concentrated by the ATHENA optics onto the focal plane. A magnetic diverter is being designed to limit the impact of these particles on the WFI background. This study will concentrate on the galactic cosmic ray background (GCR).

2.2 The Cosmic X-ray Background

The Cosmic X-ray Background (CXB) is a diffuse radiation detected over the sky in a wide range of energies from extremely soft X-rays of about 0.1 keV to γ -rays above 1 MeV. It was discovered in 1962 and its precise origin remains puzzling, although more recent observations, e.g. the deep surveys performed by ROSAT and Chandra satellites, evidenced that some fraction of the CXB is due to discrete sources (in fact more than 80 % of the CXB has been resolved in the softer range up to several keVs). Below 3 keV a Galactic component of the CXB is observed in form of thermal emission from hot gas in the Local Group. Above 3 keV the emission appears highly uniform and isotropic across the sky, suggesting that the bulk of the CXB has an extragalactic origin, though above 300 keV measurements are affected by systematic uncertainties larger than 20 %. Above 3 keV the CXB spectrum observed by HEAO-1 satellite¹² is remarkably close to the spectrum associated with thermal bremsstrahlung radiation with a temperature $kT \sim 40$ keV, whilst at energies higher than 60 keV the fit to the data requires the sum of three power laws. The Cosmic X-ray spectrum is shown on the right hand side of Fig. 1.

2.3 Production of Secondaries

The incoming background particles (henceforth called primary particles) described in the previous section interact with the whole of the ATHENA instrument and produce secondary particles. Depending on the type, energy and angular direction of these incoming primary and secondary particles, they might hit the detector and deposit energy in the 2 – 7 keV energy band, leading to background for the Wide-Field observations. In Sec. 6.2 it is shown that the bulk of the background in this energy band is generated by primary and secondary electrons and photons. While the contributing secondary electrons are mainly generated in ionization processes, the secondary photons, apart from the fluorescence photons are mainly generated in Bremsstrahlung and inelastic scattering processes.

3. GEANT4/GRAS AS TOOLS TO DERIVE THE IN-FLIGHT BACKGROUND

The simulations presented in this document have been performed using GEANT4:¹³ a general purpose Monte Carlo toolkit for elementary particles passing through and interacting with matter originally designed for high energy particle physics. GEANT4 is an open source object-oriented simulation toolkit that offers a wide set of

electromagnetic and hadronic physics models, a good performance of the particle transport in complex geometry models and the possibility of interfacing to external packages such as simulation engines and visualization or analysis tools. An effort has been made to adapt GEANT4 settings to space physics, for electromagnetic interactions a specialized physics list for space processes is used, developed in the AREMBES effort (for AREMBES GEANT4 validation see Refs. 14, 15). GRAS¹⁶ is a GEANT4-based tool that deals with common radiation analyses types in generic 3D models. Thanks to its modular design, ease of use and flexibility it is a convenient toolkit to simplify the usage of GEANT4 for space applications. The GEANT4 version used for the background studies presented in this paper is GEANT4 10.03 together with GRAS 04.00.

GEANT4 simulates the path of one incoming primary particle, its energy deposits in matter as well as the possible generation of secondary particles and their subsequent interaction with matter. The energy deposited in the sensitive detector volume in adjacent pixels by one incoming primary and its secondaries, together with the particle rate of this type of primary particle background, is used to calculate the background rate.

The physics of different particle processes are included into GEANT4 by the usage of physics lists. In a physics list the particles, physics processes and cut-off parameters to be used in the simulation are defined. The usage of physics lists allows the user to choose the best suited physics models for the energy ranges and processes in which she or he is interested. Thus, giving the user the freedom to trade physics accuracy versus computational speed. This freedom requires of the user a good understanding of the underlying physics, as an omission of particles or physics processes could cause errors or poor simulation accuracy. The physics lists used for simulations described in this document are QBBC as physics list for hadronic processes and a special physics list for space users for electromagnetic physics. The QBBC list is a readymade list of physics processes to be used for different particle and energy ranges, based on the Fritiof (FTFP) model for high energies, the Bertini (BERT) model for intermediate energies and the binary cascade model (BIC) for low energies, in addition a high precision (HP) model is used to simulate the interaction of slow neutrons. The space user physics list is a special physics list for a high precision simulation of electromagnetic processes in space physics and has been developed in the AREMBES effort.

An important parameter for the user of GEANT4 is the so called range cut, which is actually a production threshold. In GEANT4 simulations, if a process occurs in which secondary particles could be produced, the range of each secondary is checked against the range cut. Apart from some exceptions if the range of the secondary particle is smaller than the range cut it will not be produced and its kinetic energy deposited at the site of the interaction. This affects the number of low energy deposits at the detector as well as the position of energy deposits. Choosing a good range cut is a balancing act, it needs to be low enough to get the physics one is interested in but choosing it too low could lead to infrared divergence for some processes and with this a huge CPU time needed for the simulation. The default range cut used in the presented simulations is 1.0 μm . In order to emulate the particle environment, primary particles in the simulations are assumed to be emitted from a spherical surface surrounding the WFI model, with an angular cosine type input spectra. Using a cosine input spectra the fluence for each direction is proportional to the cosine of the angle between the source direction and the local normal to the sphere surface, leading to an isotropic distribution in the volume. Integrating the flux ϕ emitted with a cosine distribution over the entire surface S of a sphere with radius r yields the number of produced particles N_r in a given time frame. A factor f_N is used to normalize the simulated energy spectrum spectrum to the expected real world energy spectrum:

$$f_N = \frac{N_r}{N_S} = \phi \cdot \frac{S}{4 \cdot N_S}$$

f_N : Normalization factor

N_r : Number of expected primary particles

N_S : Number of simulated primary particles

ϕ : Flux of primary incoming particles [$\text{particles}/\text{cm}^2/\text{s}$]

S : Surface from which primary particles are emitted [cm^2]

4. EXPERIMENTAL VERIFICATION OF GEANT4 SIMULATIONS

Significant efforts have been made within the Athena WFI Background Group to validate the physics processes within the Geant4 simulation toolkit specifically for the application to instrument background generation relevant to radiation that will impact images produced by the WFI. Previous research in this area has focused on validating Geant4's simulation of particles which are well above the energies that will influence the background within the WFI.^{17–20} The off-axis X-ray-like background experienced by the WFI is expected to be primarily generated by secondary particles between several keV and several hundred keV and therefore requires specific and additional focus.

Therefore, three phases of experiments have been performed to assess the accuracy of Geant4 simulations within the context of low energy background-inducing particles in the space-based environment.²¹ Initial proof-of-concept and test phases, Phases I and II, were performed at the Synergy Health proton facility, Oxfordshire, UK using 6 MeV protons, while phase III was performed at the Proton Irradiation Facility (PIF) at the Paul Scherrer Institut (PSI), Aargau, Switzerland using 200 MeV protons to better represent the space environment. Corresponding simulations were developed for each of the experimental campaigns in order to validate Geant4's abilities to simulate X-ray-like background. Here we report on the results of the Phase III experiment which is the most relevant for the Athena WFI.

4.1 Experimental Setup

An experimental chamber was designed as shown in Fig. 2. The chamber was oriented such that protons from the PIF beamline would pass through a 2.8 cm thick plate of aluminium at 45 degrees to the surface normal such that the thickness of aluminium traversed by the beam was 4 cm, followed by two 1 mm thick targets also at 45 degrees to the beamline. Secondary particles generated by protons passing through the shield materials would then be observed by the detector without the detector being subjected to the primary beam. This geometry was designed to emulate the structure of material a cosmic proton might pass through in the space-based environment of the WFI (several centimetres of aluminium proton shield followed by two thin graded-Z shielding layers).

Figure 2. An image of the experimental chamber positioned in the beamline at the PSI Proton Irradiation Facility is shown in Fig. 2(a) and the equivalent simulated geometry is displayed in Fig. 2(b). The solenoids were used as part of the experimental programme to allow deflection of the soft electron secondaries.

Five irradiations were performed using different combinations of materials for the target, which are given in Table 1. These configurations were chosen to represent candidate materials at the time of the experiment for the WFI graded-Z shielding.

Configuration	Thickness traversed by protons
aluminium only, no graded-Z sample	4 cm Al
aluminium → molybdenum	4 cm Al → 1.414 mm Mo
aluminium → molybdenum → beryllium	4 cm Al → 1.414 mm Mo → 1.414 mm Be
aluminium → molybdenum → PEEK	4 cm Al → 1.414 mm Mo → 1.414 mm PEEK
aluminium → tungsten → PEEK	4 cm Al → 1.414 mm W → 1.414 mm PEEK

Table 1. The material configurations that were irradiated in phase III tests at the PSI Proton Irradiation Facility. As the aluminium and target material layers were oriented at 45 degrees to the beamline, the thickness traversed in each layer is equal to the actual thickness of the layer multiplied by the square root of 2.

At the time of the experiment, PEEK was one of several shortlisted materials under discussion for the baseline configuration for the low-Z shielding layer. However, the graded-Z shield is now expected to be composed of a molybdenum high-Z layer and a Kapton low-Z layer. Other simulations have demonstrated that, within the limitations those materials simulated, the choice of low-Z layer does not significantly alter the background other than modifying effectiveness at attenuating fluorescence lines.¹ It is therefore not expected that results for the actual graded-Z shielding configuration will significantly differ to the configurations with two shielding layers given here although this will be confirmed by further test campaigns in the near future.

The detector used in the experiment was a CCD97,²² an EMCCD with an approximately 14 μm thick sensitive region²³ and 512×512 pixels of width 16 μm . While this detector has a sensitive region that is significantly thinner than the WFI DEPFET sensitive region of 450 μm , it is still suitable for investigating a key component of the background, that being the secondary soft-electrons generated when a proton passes through the inner-most surfaces of the shielding materials^{1,24} as well as the fluorescence in the WFI energy band. Future experiments at the PSI PIF are currently scheduled that will use a detector with a more comparable thickness to the WFI DEPFETs, in order to test the current baseline molybdenum-Kapton graded-Z shielding configuration.

Simulations used Geant4 10.4.p01 and the corresponding version of the Space Users Physics List²⁵ built onto QBBC, with a cut length of 1 μm . Fluorescence, Auger electrons and PIXE options were also all turned on, as was single scattering, and the minimum energy was set to 100 eV. The CCD97 was modelled as a single 14 μm cuboidal block of silicon. Energy depositions in the silicon were recorded and pixelated into images, and event detection algorithms were applied to convert images to spectra.

4.2 Results

A selection of the total experimental and simulated energy deposition spectra for the irradiations are displayed in Fig. 3. Fig. 3(a) displays several of the simulation spectra plotted against the Al → Mo experimental spectrum, showing that there is little variation in the general shape of the experimental spectrum with respect to material configuration and that Geant4 spectra appear to be in good agreement with the experimental spectra above approximately 5 keV. It should be noted that the aluminium 1.49 keV fluorescence line appears in all experimental runs due to the aluminium structure of the main experimental chamber, acting as a secondary energy calibration.

Figure 3. Experimental and simulated spectra from 200 MeV proton irradiations at the PSI Proton Irradiation Facility. Fig. 3(a) shows the total energy deposition spectra for several material combinations and Fig. 3(b) shows the spectra for several configurations around the region of the 2.3 keV and 2.4 keV molybdenum fluorescence lines when the solenoids in the experiment were switched on. Fig. 3(c) and Fig. 3(d) show spectra for the aluminium only and aluminium → molybdenum configurations between 2 keV and 6 keV, and show the effectiveness of Charge Collection Efficiency (CCE) corrections at reducing discrepancies between Geant4 and experimental spectra.

There does however appear to be some divergence between the raw simulated data and that found in the experimental testing between approximately 2 keV and 5 keV in energy. As a worst case, the Geant4 simulations would appear to overestimate the electron continuum spectra by up to 50%. However, further analysis suggests that this is due, at least in the most part, to incomplete charge collection at the back surface of the CCD in the experimental data. Using data from experiments that were performed at Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung (BESSY) in Berlin on a CCD97,²⁶ a correction to simulate the incomplete charge collection at these lower energies in the experiment was applied to simulated data to give the spectra shown in Fig. 3(c) and Fig. 3(d).

The application of this charge collection efficiency correction improves the agreement between simulation and experimental data between 2 keV and 5 keV, and although it does not entirely account for the discrepancy, leaves an uncertainty related to the validity of the simulated spectra over the 2-7 keV energy band of $\sim 20\%$ when including all experimental errors. The next experimental campaign will aim to examine this discrepancy in further detail, particularly with regard to the variation between shielding candidates.

In addition to verifying the accuracy of Geant4 at simulating X-ray-like background induced by secondary particles, this experiment was also able to assess the effectiveness of graded-Z shielding at removing fluorescence lines from the background. Several solenoids were placed around the detector in a Helmholtz coil structure such that when a current was passed through the solenoids, secondary electrons would be magnetically diverted away from the detector leaving the photonic components to dominate the resulting spectra. This meant that fluorescence from molybdenum previously obscured by the electron continuum could be exposed, and the resulting spectrum when the magnetic field was switched on is displayed in Fig. 3(b). The fluorescence lines from molyb-

denum only appear in the aluminium and molybdenum only spectrum and is absent in spectra that include the beryllium and PEEK. This indicates that beryllium and PEEK are successfully attenuating the molybdenum 2.3 keV and 2.4 keV fluorescence lines, as one would rightfully expect.

4.3 Future Experiments

The results for this experiment are promising and indicate that Geant4 is capable of providing secondary particle spectra estimates accurate over a wide range of energies. In order to further validate the use of Geant4 at simulating the X-ray-like background in the ATHENA WFI, another round of testing will be performed at the PSI PIF, where the CCD97 will be replaced with a 500 μm thick AdvaPIX TPX3 detector²⁷ to better reflect the thickness of the WFI DEPFETs. The baseline graded-Z shielding configuration of a molybdenum high-Z layer with a Kapton low-Z layer will also be used in the next round of testing.

5. DESCRIPTION OF MASS MODELS USED IN GEANT4 SIMULATIONS

5.1 Baseline simplified WFI Mass Model for GEANT4 simulations

The baseline WFI simplified model (Fig. 4) used in the current simulations is derived from the WFI E00023277 CAD model. This CAD model includes the camera, thermal interface, proton shield, filter wheel and baffle. FASTRAD SW 3.9.4.²⁸ has been used to simplify the CAD model and translate it to the GEANT4 compatible GDML format. Care has been taken to model the structures close to the large detector array as accurate as possible.

5.2 Description of External Masses

The WFI camera is surrounded by several mechanical parts and structures also mounted on the Science Instrument Module (SIM). This distribution of external masses has to be taken into account in estimating the overall WFI NXB level, as secondaries can be excited from these structures, which could then reach the WFI detector. The most massive part is the X-IFU dewar, which will be mounted at a distance of 1-1.5 m from the WFI camera (Fig. 5). The dewar is mainly made of Aluminum but has a quite complex structure and contains various components and elements, as well as a lot of empty space inside. Therefore, in the simulations it has been modeled in a simplified way as a cylindrical volume, with an equivalent thickness of 70 mm and a height of 1300 mm. The equivalent thickness of Aluminum has been estimated from the energy loss of protons passing through the dewar. We discuss in Section 6.3 the results of simulations and the impact of the X-IFU dewar on the WFI non x-ray background level.

6. RESULTS OF BACKGROUND SIMULATION STUDIES

The focus of the presented studies is to minimize the anticipated background intensity. In addition fluorescence lines in the WFI energy observation range should be prevented as far as possible. Special care has been taken to understand the systematic uncertainties due to variations of the WFI design and surroundings. In order to find the best graded Z-shield in terms of choice of materials and their thicknesses a simplified model has been used. In this way many different configurations could be simulated in an acceptable time frame. This optimization process is described in Sec. 6.1. Based on the outcome of this optimization, the simplified WFI mass model described in Sec. 5.1 has been modified. In Sec. 6.2 an estimate of the background for this modified WFI baseline model is given. Sec. 6.3 shows the deterioration of WFI's background level if additional masses of the ATHENA spacecraft, in the vicinity of WFI, like X-IFU, the magnetic diverter, and the instrument platform are taken into account. In addition to the graded Z-shield on the inside of the camera head further parts of the WFI can be shielded to reduce fluorescence lines. In Sec. 6.4 the remaining fluorescence counts for different shielding decisions are presented. Sec. 6.5 discusses how, based on the simulation results, a technical feasible low Z graded-shield material has been found. A note on the employment of software rejection algorithms for background reduction is given in Sec. 6.6.

Figure 4. ATHENA's WFI instrument. (a) Detailed CAD model, including Camera, Proton Shield, Filter Wheel and Baffle. (b) Simplified model used as baseline model for current GEANT4 simulations, presented in 5.1. (c) Cross-section through detailed CAD model of camera head. (d) Cross-section through simplified baseline model for current GEANT4 simulations. Directly in the center, marked in turquoise, is the large detector array with its four DEPFET detectors. Aluminum structures are shown in silver, molybdenum structures in green, silicon structures in blue and kapton structures in pink.

6.1 Optimizing the Graded Z Shield on Simplified Model

The first phase of the study on the WFI non x-ray background (NXB) had led to the conclusion that an inner shield should be adopted inside the Al bulk shield to conveniently reduce the secondary emission from the bulk towards the detector as well as improve the bulk stopping power against environmental hard x-ray photons (see Ref. 1). As a preliminary and tentative baseline an inner shield consisting of a bilayer with 1 mm Mo and 1 mm PEEK was considered, as a good compromise between desired performance and realistic possibility of technical implementation. Nevertheless, the corresponding overall NXB level, as simulated using mass model E00015261, still was $\sim 30\%$ higher than the requirement, also due to the contribution from secondary emission from external masses (namely the XIFU cryostat, see Sec. 6.3) around the WFI camera. In order to improve the configuration design, the initially adopted approach was to run systematically GEANT4 (G4) simulations on the basic geometry model, which requires less computational power and time, varying the shield parameters and exploring different combinations of them, and do verification and confirmation of the results with a more complete and detailed mass model just for those combinations showing some clear benefits in terms of NXB level.

Figure 5. Schematic view of the WFI camera and X-IFU dewar on the SIM.

In a first round of simulations the baseline materials, Aluminum, Molybdenum and PEEK have been assumed and just variation of their thicknesses has been investigated. During this stage of the analysis, PEEK, has been considered a prime candidate for the low Z layer, Technical feasibility considerations have, in a later stage, lead to Kapton as prime candidate. As a first step, the thickness of Molybdenum has been increased while keeping constant the thickness of PEEK, in order to assess how much reduction of the fraction of NXB induced by cosmic x-ray background (CXB) could be achieved. The larger the Molybdenum thickness the higher the photon rate attenuation. On the other hand, if the Molybdenum thickness becomes too large, secondary particle generation, excited by charged particles in the Molybdenum, could overcompensate this effect. Also, the larger the Molybdenum thickness the larger the weight, which should be kept within a reasonable limit. For this reason, only three different cases have been investigated: 3 mm Mo, 5 mm Mo and 7 mm Mo (plus 1 mm PEEK in all three cases). Simulations showed that some improvement of the overall NXB can be achieved, with 3 mm Mo and 5 mm Mo performing slightly better than 7 mm Mo (see Table 2).

Input particle	Configuration 1	Configuration 2	Configuration 3
GCR protons	+2.7 % $\pm$ 3.2 %	+5.9 % $\pm$ 4.2 %	+8.8 % $\pm$ 4.1 %
GCR He-ions	-9.2 % $\pm$ 5 %	-11.5 % $\pm$ 5.1 %	-2.2 % $\pm$ 5.1 %
GCR electrons	-3.1 % $\pm$ 7.4 %	-8.2 % $\pm$ 7.5 %	-11.7 % $\pm$ 7.9 %
CXB photons	-67.3 % $\pm$ 1.4 %	-80.2 % $\pm$ 1.1 %	-85.8 % $\pm$ 0.8 %
All primary particles	-10.1 % $\pm$ 3.7 %	-10.5 % $\pm$ 4.6 %	-9.6 % $\pm$ 4.6 %

Table 2. Summary of NXB relative variation (wrt. configuration 0) for different input particles and configurations. Configuration 0 = 40 mm Al + 1 mm Mo + 1 mm PEEK. Configuration 1 = 40 mm Al + 3 mm Mo + 1 mm PEEK. Configuration 2 = 40 mm Al + 5 mm Mo + 1 mm PEEK. Configuration 3 = 40 mm Al + 7 mm Mo + 1 mm PEEK

As a second step, assuming a thickness of 3 mm Mo, the PEEK thickness has also been changed to see whether any further improvement could be achieved. Four cases have been investigated: 0.125 mm, 0.25 mm, 0.5 mm and 1.5 mm. Simulations showed that the thickness of PEEK is useful to suppress Mo fluorescence lines but does not affect significantly the continuum level. In fact, the mean values of NXB in the 2-7 keV range resulted quite similar to each other, within statistical errors, as reported in Table 3.

Similar simulations have been then repeated replacing PEEK with other possible alternative low-Z materials suitable for implementation, namely Kapton and Polypropylene. Even in this case, the simulations indicated only minor differences, the three candidate materials behave in a similar way and can be considered interchangeable in terms of associated NXB. As an example, in Table 4 the relative variations are compared for a layer with a thickness of 0.125 mm.

PEEK thickness	NXB relative variation
0.125 mm	-7.2 % $\pm$ 2.6 %
0.25 mm	- 5.1 % $\pm$ 2.6 %
0.5 mm	-3.5 % $\pm$ 2.9 %
1 mm	-4.6 % $\pm$ 2.9 %
1.5 mm	-2 % $\pm$ 2.9 %

Table 3. Summary of NXB relative variation (wrt. a configuration with 40 mm Al + 3 mm Mo w/o PEEK layer) for different thicknesses of the PEEK layer.

Material (0.125 mm)	NXB relative variation
PEEK	-7.2 % $\pm$ 2.6 %
Kapton	-6.5% $\pm$ 2.6 %
Polypropylene	-8.9% $\pm$ 2.6 %

Table 4. Summary of NXB relative variation (wrt. a configuration with 40 mm Al + 3 mm Mo w/o low-Z layer) for a 0.125 mm layer of PEEK, Kapton and Polypropylene.

Furthermore, a configuration with a reduced thickness of the Aluminum bulk shielding (i.e. 30 mm instead of 40 mm) has been investigated as well, since the proposed increase in the Mo layer thickness would even offer an extra protection against radiation damage. A decreased Aluminum thickness leads to more background induced by CXB and cosmic electrons. Reducing the Aluminum thickness from 40 mm to 30 mm increases this background contribution by ~ 20 %. However, decreasing the Aluminum thickness, leads on the other hand to less background due to secondary particles induced by cosmic protons and He-ions, which compensates the CXB and cosmic electron contribution. It has been found that within errors both Aluminum thicknesses, 30mm and 40mm, can be considered equivalent.

In conclusions, the findings of the study conducted on the basic mass model can be summarized as follows: increasing the thickness of the inner layer of Mo from 1 mm to 3 mm or 5 mm would allow to gain ~ 20 % reduction in the overall NXB. Even though in these simplified simulations a thickness of 5 mm Mo seems to work slightly better than a thickness of 3 mm, the latter one could be preferable in order to keep the layer weight as low as possible; an increased thickness of the inner layer of Mo would also offer an extra protection against radiation damage, which would allow to reduce then the thickness of the Al bulk shield from 40 mm to 30 mm without any significant impact on the overall NXB level. According to simulations, the composition and thickness of the inner low-Z layer does not affect significantly the overall continuum level. In this case, the choice of material thickness and composition could be driven by other properties of the material e.g. mechanical stability, outgassing, etc., provided that a low Z layer thickness sufficient to fully suppress the Mo fluorescence L-line is used.

6.2 Simulated WFI Background with Optimized Baseline Model

Using the outcome of the graded Z-shield study, presented in Sec 6.1 and the results of previous studies,¹ the following changes have been made to the baseline WFI model presented in Sec. 5.1. The proton shield in the optimised model has been reduced from 4 cm thickness to 3cm thickness. In order to compensate the resulting loss in radiation protection and to suppress secondary and primary photons a 3 mm thick Molybdenum layer together with 1 mm of PEEK are included as graded z-shield inside of the proton shield. The low Z PEEK layer suppresses the resulting aluminum and molybdenum fluorescence lines. In the baseline shielding model, the inside of the detector opening in filter wheel and primary structure are as well coated by 1 mm of PEEK. This low Z PEEK layer, used in GEANT4 simulations described in this section, stands in contrast to the low Z Kapton layer described in Sec. 1.1. This is due to the fact, that the graded Z-shield composition described in Sec. 1.1 is an outcome of these simulations plus a technical feasibility study.

The resulting background is presented in Fig. 6. The different shape of background due to cosmic ray photons and cosmic particles is clearly visible. While the particle background is relatively flat in the regarded energy range the photon background increases with decreasing energy. This is confirmed in Table. 5, which presents the best fitting parameters of 1 dimensional polynomials for the particle background spectra and a 2 dimensional polynomial for the photon background spectra. A chi2 criteria has been used to find the appropriate polynomial

Figure 6. Instrumental background spectra due to cosmic protons (red), electrons (magenta), He-ions(green), photons(blue) and the sum of all (black). The simulation results were derived for the proposed optimized WFI configuration, including a Mo/PEEK graded Z-shield. No rejection algorithms have been employed.

degree for the different background spectra. Fig. 6 shows clearly the Aluminum K alpha line. More information on fluorescence lines is given in Sec. 6.4.

Primary particle	p0 $\cdot 10^{-3} [\text{cts}/\text{cm}^2/\text{s}/\text{keV}]$	p1 $\cdot 10^{-3} [\text{cts}/\text{cm}^2/\text{s}/\text{keV}^2]$	p2 $\cdot 10^{-3} [\text{cts}/\text{cm}^2/\text{s}/\text{keV}^3]$
GCR protons	4.8 ± 0.1	-0.02 ± 0.02	-
GCR He-ions	0.43 ± 0.04	-0.003 ± 0.004	-
GCR electrons	0.58 ± 0.04	0.007 ± 0.004	-
GR photons	0.83 ± 0.06	-0.10 ± 0.01	0.0037 ± 0.0007

Table 5. Polynomial coefficients of a 1 dimensional polynomial fit to the different particle background curves and a 2 dimensional polynomial fit to the cosmic photon background. Fitting region 2 - 15 keV.

The mean background level between 2 and 7 keV is presented in Table 6, in the first column without any additional software rejection algorithms, in the second column all hits touching the detector borders have been excluded and in the third column a 20% margin has been added to the mean background level to account for simulation uncertainties. Without further cleaning processes the background is not compatible with the requirement stated in Sec. 1.2.

Fig. 7 shows on the left hand side the fractional background contribution of the main primary particle and on the right hand side the fraction background contributions of particles impinging on the detectors. Galactic cosmic protons contribute approximately three quarters of the background, the rest is split almost evenly between cosmic He-ions, cosmic electrons and cosmic unfocused photons. The background is mainly generated by electrons and photons impinging on the WFI large detector-array.

6.3 Effect of External Masses on Background

The assessment mainly concerns the impact of the presence of the X-IFU dewar, which is the most massive structure in the vicinity of the WFI camera, on the NXB level expected for the WFI detector and was initially conducted using mass model E00015261.⁷ The dewar has been modeled in a simplified way as equivalent to a cylinder made of Al with inner radius 400 mm, outer radius 470 mm and height 1300 mm. Simulations have

Primary particle	Mean Bkgd. $\cdot 10^{-3}[\text{cts}/\text{cm}^2/\text{s}/\text{keV}]$	Mean Bkgd. excl. border hits $\cdot 10^{-3}[\text{cts}/\text{cm}^2/\text{s}/\text{keV}]$	Mean Bkgd. excl. border hits + syst. unc. $\cdot 10^{-3}[\text{cts}/\text{cm}^2/\text{s}/\text{keV}]$
GCR protons	4.81 ± 0.08	4.68 ± 0.08	5.62 ± 0.08
GCR He-ions	0.49 ± 0.03	0.49 ± 0.03	0.59 ± 0.03
GCR electrons	0.66 ± 0.02	0.64 ± 0.02	0.77 ± 0.02
GCR photons	0.48 ± 0.02	0.48 ± 0.02	0.58 ± 0.02
Total	6.44 ± 0.09	6.29 ± 0.09	7.54 ± 0.09

Table 6. The mean simulated particle background level between 2 and 7 keV for different incoming particles in $\text{cts}/\text{s}/\text{cm}^2/\text{keV}$. The first row shows the full uncleaned background, the second row the background if hits touching the detector border are removed, the third row the adds a safety margin to the background after the first cleaning.

Figure 7. Fractional contribution to mean background level between 2 and 7 keV, (a) split according to the primary particle species and (b) split according to the particles species hitting the detector.

been run for all primary particles both with and without dewar. The comparison showed that the presence of the dewar introduces an additional radiative component in form of secondary gammas, which are generated as a consequence of hadronic interactions of primary charged particles in the dewar mass. These gammas leave the dewar and have enough energy to penetrate through the Al bulk shield of WFI and reach the detector, where they do contribute to the NXB via Compton scattering. While all charged particles excite secondaries in the dewar mass and generate some additional emission (mostly stopped by the Al bulk shield), for CXB photons the presence of the dewar has just the effect of reducing the solid angle and preventing then a fraction of the incoming flux from reaching the detector. The overall NXB variation associated with the dewar in the mass model version E00015261 resulted $+12.3\% \pm 6.7\%$.

Similar simulations have been then repeated following the evolution of the WFI camera design as well as the SIM design. In particular, in Table 7 we report quantitatively the relative variation of NXB for each type of primary input particle simulated using the latest mass model version E00023277, where the shielding structure consists of 30 mm Al + 3 mm Mo + 1 mm PEEK. According to an updated SIM design, with respect to former simulations the distance between the dewar and the WFI detector has been increased from 1.1 m to 1.4 m.

Although the shielding composition is not the only difference between the mass models E00015261 and E00023277, it is reasonable that the increased thickness of the Mo layer from 1 mm to 3 mm together with the larger distance between the WFI camera and the dewar more than compensate the reduction of thickness of the Al bulk shield from 40 mm to 30 mm, then resulting in a lower additional NXB from the dewar for the mass model E00023277. It is worth stressing that since the additional NXB is mainly associated with secondary energetic gammas, which can easily penetrate through a thin low-Z layer, we expect that replacing PEEK with a different low-Z material (e.g. Kapton) in the same E00023277 mass model version does not have a significant impact on the result.

Input particle	NXB mean variation
GCR protons	+6.1 % $\pm$ 3.2 %
GCR He-ions	+18.4 % $\pm$ 10.1 %
GCR electrons	+4.9 % $\pm$ 3.7 %
CXB photons	-9.6 % $\pm$ 9.9 %
All primary particles	+5.9 % $\pm$ 4.3 %

Table 7. Summary of NXB mean variation in 2-7 keV for different input particles mainly induced by secondary gammas in a configuration including the WFI mass model E00023277 plus the X-IFU dewar, relative to the NXB simulated for the mass model E00023277 w/o dewar.

6.4 Effect of Varying the Shielding Configuration on Fluorescence Photon Counts

Three different shielding configurations have been tested.

ID 0: Baseline configuration: A full graded z-shielding inside of the camera head (3 mm Molybdenum and 1 mm PEEK), and 1 mm PEEK shielding on the inside of the detector opening of the primary structure.

ID 1: A full graded z shielding on the inside of the camera head but no other graded z shielding.

ID 2: A full graded z shielding on the inside of the camera head and 1 mm PEEK shielding on the inside of the WFI baffle walls, no shielding on the inside of the detector opening of the primary structure.

For baffle and primary structure no Mo shielding has been considered for the following reasons.

1. The aluminum layer of the primary structure surrounding the detector opening is thin (a few mm), therefore the number of Bremsstrahlungsphotons generated in this layer should be few. Adding a Molybdenum layer would lead to more Bremsstrahlungsphotons and hence background.
2. An additional Molybdenum layer on these thin parts would increase the overall weight of these extended components and could critically affect the structural integrity of the WFI.

The resulting Aluminum K photon background hits and Molybdenum L photon background hits are presented in Table 8. The lowest amount of Aluminum K photon background hits can be observed with the baseline shielding configuration ID 0. Further reduction to $\sim 0.3 \pm 0.1$ cts/cm²/s would be possible if in addition to the ID0 shielding baffle walls could be shielded with a low Z material. This number has been estimated by subtracting from the Aluminum K photon counts, photons emitted from the baffle walls. The technical feasibility of shielding the baffle walls is currently under discussion. Also for reduction of Molybdenum L photons shielding configuration ID 0 is the best choice of the three. Only very few Molybdenum L photons remain. The origin of Aluminum L photons and Molybdenum K photons for shielding configuration ID 1 is shown in Fig. 8. The majority of the Aluminum K line photons originate from the primary structure and the filter wheel. This is due to an incomplete low Z shielding of these structures. The overall aluminum count could therefore be further reduced, if a complete low Z shielding of these structures would be possible. The majority of the Molybdenum L line fluorescence photons originate from the detector holder, directly adjacent to the detector. Attaching a low Z shielding here is particularly difficult due to thermal stress and closeness of the detector. The detector holder will be cooled together with the detector, this would induce thermal stress into a low Z layer attached to the inside of the detector holder. In order to reduce risks to the detector a low Z layer on the inside of the detector holder is therefore not foreseen and also according to the simulations not strictly necessary.

Shielding configuration	Aluminum K photons $\cdot 10^{-3}$ [cts/cm ² /s]	Molybdenum L photons $\cdot 10^{-3}$ [cts/cm ² /s]
ID 0	0.7 ± 0.1	0.3 ± 0.1
ID 1	2.5 ± 0.1	0.6 ± 0.1
ID 2	2.0 ± 0.1	0.5 ± 0.1

Table 8. Aluminum K and Molybenum L line fluorescence photon hits.

Figure 8. Origin of fluorescence photons hitting the detector for shielding configuration ID 1. (a) The origin of aluminum K line photons, (b) the origin of molybdenum L line photons. The detector-holder is the molybdenum structure marked in green in Fig. 4.

6.5 Technical Feasibility of Graded Z-shielding

The graded Z shield studies presented in the previous sections assumed that the lower Z layer would consist of 1mm of PEEK. Regarding the technical feasibility, with respect to out-gassing, stability, availability and thermal requirements the choice of a suitable lower Z layer is much more limited. The current best choice of a lower Z layer would be, as stated in Sec. 1.1, 40 μm of kapton glued with epoxy adhesive to the molybdenum high Z-layer. The foreseen kapton is the material with the maximum available thickness which fulfills the required standards in out-gassing, stability, positive thermal influence, grounding and space qualification. Simplified background simulations have been used to estimate if this thickness suppresses sufficiently the Molybdenum K line. In these simulations an epoxy thickness of 100 μm has been assumed, which is in accordance with standard epoxy thicknesses for similar applications. The resulting Molybdenum K line photon count should be in the same order of magnitude as that stated in Table 8 for ID 0. Using a 3 cm Aluminum, 3 mm Molybdenum box model (from outside to inside), with inner and outer volumes similar to the WFI camera head, the unsuppressed number of Molybdenum L photons has been estimated. Together with the transmission efficiencies for Polyimide and Polyether (hendke) the remaining Molybdenum K photons have been calculated for several low Z layer variations (Table 9). All estimated remaining Molybdenum K photon counts are one order of magnitude lower than those expected for shielding configuration ID0, which are mainly emitted from the Molybdenum detector holder. A change from the 1mm PEEK thickness in shielding ID 0 to 40 μm of Kapton glued with ca. 100 μm Epoxy should therefore have negligible effects on the overall expected Molybdenum K photon count.

Shielding configuration	Molybdenum K photons $\cdot 10^{-5} [\text{cts}/\text{cm}^2/\text{s}]$
80 μm Kapton	4.6
125 μm Kapton	1.0
250 μm Kapton	0.01
40 μm Kapton 100 μm Epoxy	0.9

Table 9. Molybenum L line fluorescence photon hits for different thicknesses of a low Z layer and a possible adhesive thickness using a simple box model simulation.

6.6 Effectivity of Rejection Algorithms

As pointed out above, further reduction of the background level can be achieved through software rejection. In order to reduce the remaining background several analysis strategies have been tested. One of them is the exclusion of hits which are next to a pixel in which more than 15 keV of energy have been deposited (overflow

pixel) during one integration time. The reasoning behind this threshold is that energy deposits above 15 keV are much more likely to originate from high energetic particles than from X-ray photons which have been focused by the mirror onto the detector. Secondary particles produced by such a high energetic primary tend to hit the detector close to the primary which produced them. This is especially true if the secondaries are produced on a surface parallel and close to the detector. The closest distance between a background hit and an overflow pixel is depicted in Fig. 9 for galactic cosmic ray protons only. Two separate distributions can be seen, one peaking at small distances and one almost flat reaching up to large distances. The current assumption is, that the first distribution is due to secondaries produced on a surface close and parallel to the detector, while the second distribution is due to secondaries produced further away from the detector or from secondaries due to unrelated primaries arriving during the same frame time. It is important to understand that this technique is limited to frames in which more than one hit has been detected. An in depth discussion of software rejection algorithms can be found in Ref. 29.

Figure 9. Smallest distance between background hit and overflow pixel in number of pixel for galactic cosmic protons as primary particles.

7. WFI BACKGROUND SUMMARY

The overall background level is given in Table 10, including the removal of hits touching the detector border, the inclusion of the effect of external masses like the XIFU dewar and taking into account systematic uncertainties on the GEANT4 simulation process. This systematic uncertainties have been estimated to be about 20%. The final level, adding systematic uncertainties, is about 45% higher than the total required focused and not-focused instrumental background level given in Sec. 1.2. Based on extensive simulation studies we come to the conclusion that this is the best background achievable for the WFI DEPFET detectors at L2, if no further software rejection algorithms are employed. In Ref. 29 possible software rejection algorithms are discussed. The goal is to find a rejection algorithms which optimizes the overall signal over background level.

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Primary particle	Mean Bkgd. - border hits + external masses $10^{-3}[\text{cts}/\text{cm}^2/\text{s}/\text{keV}]$
GCR protons	4.97 ± 0.08 (stat) ± 1.0 (syst)
GCR He-ions	0.58 ± 0.03 (stat) ± 0.1 (syst)
GCR electrons	0.67 ± 0.02 (stat) ± 0.1 (syst)
GCR photons	0.45 ± 0.02 (stat) ± 0.09 (syst)
Total	6.7 ± 0.1 (stat) ± 1.3 (syst)

Table 10. The mean simulated particle background level between 2 and 7 keV for different incoming particles in $\text{cts}/\text{s}/\text{cm}^2/\text{keV}$. The second column shows the background after removal of hits touching the detector border and taking into account external masses. Statistical errors correspond to the 1σ error on the mean, systematic error account for a 20% uncertainty in the modelling of the WFI and surrounding and for uncertainties inherent in GEANT4 simulations.

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