Exp Astron (2017) 44:401–411
DOI 10.1007/s10686-017-9537-2

ORIGINAL ARTICLE

A revision of soft proton scattering at grazing incidence and its implementation in the GEANT4 toolkit

Alejandro Guzmán[1] · Emanuele Perinati[1] · Sebastian Diebold[1] · Chris Tenzer[1] · Andrea Santangelo[1]

Received: 18 January 2017 / Accepted: 8 May 2017 / Published online: 15 August 2017

Abstract The scattering of soft protons inside the Wolter-type optics of X-ray observatories has been proven to concentrate these particles onto the focal plane instruments. The funneling of these protons increases the instrumental background and can also contribute to the degrading of the detectors. The instrumental background and degradation of the detector's performance experienced by Chandra and XMM-Newton is significantly larger than what was expected on the basis of previous Monte Carlo simulations. For Chandra the main issue is the degradation of the energy resolution due to lattice displacements in the detectors. For XMM the contribution to the instrumental background is more significant. In between, new laboratory measurements as well as a revision of the theory are needed to correctly assess the impact of the environmental radiation for future missions. In this publication we present a GEANT4 class that will allow future users to select between either theoretical models or measured data to simulate the scattering of soft protons at grazing angles. To develop this method, we revisit the theory of elastic scattering of protons on polished surfaces and implement these approaches into GEANT4. We also implemented recently performed measurements using parts of *eROSITA* (extended ROentgen Survey with an Imaging Telescope Array) mirror shells as scattering targets as another scattering model to be used within the GEANT4 toolkit.

Keywords Grazing angle protons · X-ray Optics · X-ray space observatories · Simulations

✉ Alejandro Guzmán
guzman@astro.uni-tuebingen.de

[1] Institut für Astronomie und Astrophysik Tübingen, Sand 1, 72076 Tübingen, Germany

1 Introduction

The evidence that soft protons in the space environment may be focused through an X-ray telescope emerged after the launch of the X-ray observatory Chandra: once in orbit, the front-illuminated CCDs of the ACIS camera showed a worse performance than expected, while the back-illuminated CCDs worked according to their nominal specification parameters [6]. It was understood that during passages within the radiation belts the front-illuminated CCDs suffered an excess of non-ionizing energy loss (NIEL) from soft protons focused onto them by the telescope. They caused a degradation of the Charge Transfer Efficiency (CTE), since for protons of energy of the order of 100 keV the large-scale displacement damage induced by NIEL occurs just below the highly sensitive gate region at the detector surface. The understanding of the origin of the degradation for Chandra allowed to limit the same degradation on the European observatory XMM-Newton, which was launched a few months afterwards to a similar highly elliptical orbit [5]. In fact, for safety reasons it was decided to keep the EPIC camera in closed position below about 45,000 km, where the bulk of the radiation belt is found. However, soft protons present at higher altitudes still have an impact on the XMM background, which shows a flaring component in both the EPIC front-illuminated (MOS) and back-illuminated CCDs (PN) [3]. The origin of these transients is still debated, as in many cases they seem not directly associated to solar activity events. For the events not associated to solar activity, one proposed scenario is that XMM encounters from time to time clouds of soft protons randomly distributed within the magnetosphere, some of which are concentrated to the focal plane by the mirror shells producing a sudden fluctuation of the background countrate over time-scales as short as a few seconds, indicating that the density of soft protons can vary quickly within a few kilometers. Although the soft proton fluxes in space can be highly variable and there are regions, such as L2, where there is no direct information at all due to the lack of particle monitors operating in the softer energy range (i.e less than a few MeV), it is important to assess the mechanism of proton scattering at grazing incidence in order to enable more reliable predictions for future X-ray astronomy missions. In these missions the issues related to soft protons will become even more serious if larger apertures are used. The general approach for the characterization of the instrumental background in modern astrophysics is based on simulations performed in GEANT4 [1]. The aim of this work is to develop a specific class for the simulation of the soft proton scattering at grazing incidence, which is intended to upgrade the already existing description based on the classical multiple scattering processes, which seem unable to correctly reproduce the experimental measures available in literature. For this purpose, we based our class on the Remizovich's theory [7], which proposes a more complete description of the propagation of protons and ions in both the polar and azimuthal scattering directions under grazing incidence. As a validation or just as an alternative option for the user, our class also offers the opportunity to switch to a description fully based on interpolation of experimental data taken at the 3 MV Van-de-Graaff accelerator of the Institute for Physics in Tübingen, where an experiment to measure the reflectivity at grazing incidence of soft protons and ions on X-ray mirror shells from the eROSITA mission has been setup [2].

We begin in Section 2 by making a short summary of Remizovich's [7] and Firsov's [4] analytical results, presenting them with the same geometrical conventions of the measurements made in the Tübingen accelerator facility. In Section 3 we describe the insertion of said models into the GEANT4 toolkit and show the control parameters available to the user. In Section 3.1 we show the results of Monte Carlo (MC) simulations of an experimental setup similar to the one used in [2] using the new class described in this publication.

2 Summary of Remizovich's analytical solution

In the following we will be discussing the scattering of protons impinging with a grazing angle onto a metallic surface (the target). We assume the beam to be propagating in the z-direction and that the origin of coordinates is at the impact point of the beam on the target. In this system of reference the orientation of the target is inclined at an angle Ψ_0 to the zx-plane, hence the beam's incidence angle is also Ψ_0. Our convention is illustrated in Fig. 1. In this convention, the scattered particle's direction forms an angle θ (polar angle) with the zx-plane and its projection onto the zx-plane forms an angle χ with the z-axis. This system of reference is the same one that is used in the experiments at the Tübingen facility discussed in [2].

Since we will begin by stating the results presented by Remizovich et al. [7], it is necessary to introduce the adequate geometrical identifications to match up both conventions. In [7] the xy-plane coincides with the target's surface, and the z-axis extends inside the target. The main difference with our convention is that in the mentioned publication the target defines the xy-plane, which results in a different convention for the angles. This both conventions are easily reconciled by making the following identifications:

$$\begin{pmatrix} \Psi_0 \\ \theta - \Psi_0 \\ \chi \end{pmatrix}_{\text{Tübingen}} \leftrightarrow \begin{pmatrix} \zeta_0 \\ \zeta \\ \varphi \end{pmatrix}_{\text{Remizovich}}$$

Remizovich et al. solve the transport equation for the density of a particle flux propagating at a certain depth inside a dense medium (target). The scattered particles emerge from the target in the direction given by $(\theta - \Psi_0, \chi)$ and have an energy E. The other parameters relevant for the transport equation are the average energy loss per unit path $\varepsilon(E)$ and the mean-square of the scattering angle of ions by the target atoms $\langle \upsilon^2(E) \rangle$. These last two parameters are material and energy dependent. To solve this equation, Remizovich et al. make the assumption that the incidence angle, although small, is still much bigger than the scattering angle υ:

$$\upsilon \ll \Psi_0$$

The second assumption is that a particle with energy E travels a path $L(E)$ given by:

$$L(E) = R_0 - R(E) = \int_E^{E_0} \frac{dE'}{\varepsilon(E')}$$

where R_0 is the range of the particle with energy E_0.

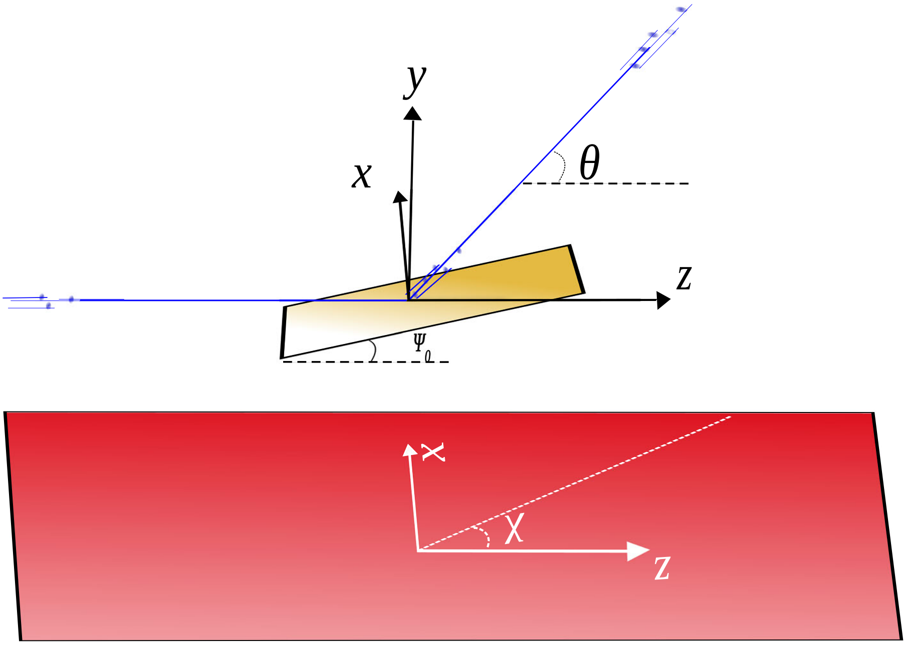


Fig. 1 The geometrical system of reference used in this work. The incoming beam of particles has the same direction as the z-axis, while the surface of the target is at an angle ψ_0 with the z-axis. The scattered particles follow a trajectory that makes an angle θ with z-axis

The solution is expressed in terms of the following dimensionless variables to simplify the notation:

$$\Theta = \frac{\theta - \Psi_0}{\Psi_0}, \qquad X = \frac{\chi}{\Psi_0}, \qquad s = \frac{L(u)}{R_0}, \qquad u = \frac{E}{E_0}$$

and a parameter which relates the ratio of mean-square value of the scattering over the whole path to the square of the glancing angle:

$$\sigma = \frac{R_0 \langle \upsilon^2(E_0) \rangle}{4\Psi_0^2}$$

Given the appropriate boundary conditions, (normalization, assuming a mono-energetic incident beam, etc.) Remizovich et al. arrive at the differential back-scattering coefficient $W(\Theta, X, u)[sr^{-1}]$, given by:

$$W(\Theta, X, u) = \frac{\sqrt{3}}{2\pi^2} \frac{E_0}{\varepsilon(u)} \frac{\Theta}{R_0} \frac{e^{-\frac{\Theta^2 - \Theta + 1}{\sigma s(u)}} e^{-\frac{X^2}{4\sigma s(u)}}}{\sqrt{\sigma^3 s^5(u)}} \mathrm{Erf}\left(\sqrt{\frac{3\Theta}{\sigma s(u)}}\right) \tag{1}$$

In this last expression we see that, for the azimuthal angle $X = \frac{\chi}{\Psi_0}$, the behavior is a gaussian centered around $X = 0$. Whereas the dependence on $\Theta = \frac{\theta - \Psi_0}{\Psi_0}$, though dominated by the gaussian, is a bit more complicated. The error function term regulates the size and the position of the maximum. The latter is in turn controlled by the product $\sigma s(u)$. Therefore, many parameters are dependent on the material. This makes it rather difficult to test its validity experimentally. Also it must be noted that Remizovich et al. do not impose any periodicity in the angular variables, but they do allow them cover the whole range $(-\infty, \infty)$.

If we integrate (1) in both energy and azimuthal angle and then take the limit as $\sigma \rightarrow \infty$, we reproduce Firsov's results for the polar angle [4]. This distribution which corresponds to a purely elastic collision with no deceleration of the particles. This is the first analytical model which we implemented in our GEANT4 class: the normalized version of Firsov's distribution, which in our original variables yields:

$$\mathscr{F}(\theta) \equiv W_{el}(\theta) = \frac{3}{2\pi\Psi_0}\left(\frac{(\Psi_0(\theta-\Psi_0))^{\frac{3}{2}}}{\Psi_0^3+(\theta-\Psi_0)^3}\right) \tag{2}$$

We proceed in a similar fashion with Remizovich's elastic distribution for both angular variables. If we write it down using this article's varibale convention we arrive at the second analytical result we implemented in GEANT4:

$$\mathscr{R}(\theta,\chi) \equiv \frac{1}{12\pi^2\Psi_0\sqrt{\Psi_0(\theta-\Psi_0)}}\left[\frac{\omega^4}{1+\omega^2}+\omega^3\text{atan}(\omega)\right] \tag{3}$$

where ω is defined to be:

$$\omega \equiv \sqrt{\frac{3(\theta-\Psi_0)\Psi_0}{(\theta-\Psi_0)^2-(\theta-\Psi_0)\Psi_0+\Psi_0^2+\frac{\chi^2}{4}}}$$

We show the two-dimensional plot of $\mathscr{R}(\theta,\chi)$ evaluated at $\psi_0 = 0.33°$ in Fig. 2.

For completeness, in Fig. 3 we plot a comparison between the Tübingen measurements and the values predicted using (3) for different inclination angles. The measurements were done with a detector which covered a limited range in the azimuthal and polar angle. For this purpose, we integrated (3) around $\chi = 0 \pm 0.03°$ and $\theta = \theta_m \pm 0.03°$, where θ_m is the measured scattering angle.

3 Implementation in GEANT4

We have created a new *VDiscreteProcess* within the GEANT4 toolkit [1]. It is based upon GEANT4's *G4OpBoundaryProcess* and its name is *G4GrazingAngleScattering*. As with any discrete process inside GEANT4 the particle's trajectory is modified after the current step. Before invoking the scattering process, our class process checks for a transition coming from a vacuum-like environment and, if this is the case, then the scattering takes place. If the latter was not the case, the particle propagates freely (unless some other GEANT4 process takes effect). The encapsulation of our scattering process in a single class is in agreement with the object oriented programming paradigm, upon which GEANT4 is conceived.

We implemented the models mentioned in the previous section (3) and (2), plus a simple linear interpolation to measurements carried out at the accelerator of the Institute for Physics in Tübingen [2]. We shall simply refer to this linear interpolation as the Tübingen model. If the Tübingen model is being used but the energy or the incidence angle of the incoming particle are beyond the measured values the model reverts to the Firsov model, to avoid nonphysical results.

To use our class, the user only needs to add the process to the user's physics list, and use the class's constructor with the suitable parameters. These parameters are listed and explained below:

- **Scattering model (integer)**. An index whose value selects which scattering model to use, it goes from 0 to 2, and selects Firsov, Remizovich, or Tübingen accordingly.
- **Maximum incidence angle [deg]**. The *G4GrazingAngleScattering* process will only scatter particles whose incidence angle to the normal of the surface is less than this value. If the incidence angle is larger, then our class carries out no scattering, thus allowing particles to penetrate the material unless some other scattering is also activated.
- **χ mean angle [deg]**. For the Firsov and Tübingen models a scattering in the *xz*-plane is also provided via a simple gaussian. The mean of the gaussian distribution is set by this parameter. It is ignored in case the Remizovich model is used.
- **χ standard deviation angle [deg]**. For the Firsov and Tübingen models a scattering in the *xz*-plane is also provided via a simple gaussian. The standard deviation (σ) of the gaussian distribution is set by this parameter. This parameter is ignored in case the Remizovich model is used.

—Example usage of the G4GrazingAngleScattering class—

```
// Set the initial values for the parameters
G4ParticleDefinition* particle // This pointer should not be a
NULL pointer
G4int model= 0 ;// Can be 0-2 (Firsov, Remizovich or Tübingen
measurement)
G4double MaxIa=1.5 ;//Maximum incidence angle (in degrees).
G4double mean =0. ;//Mean of the chi distribution (in degrees)
G4double sigma=.01 ;//Standard deviation of the chi distribution (in
degrees)
// Add the process
G4GrazingAngleScattering* gasc = new
G4GrazingAngleScattering("GrazingAngleScattering",model,
MaxIa,mean,sigma);
ph->RegisterProcess(gasc, particle);// ph is a pointer to a
PhyisicsHelper Class
```

Before we continue with our preliminary results, we would like to point out two key consequences of selecting the completely elastic case:

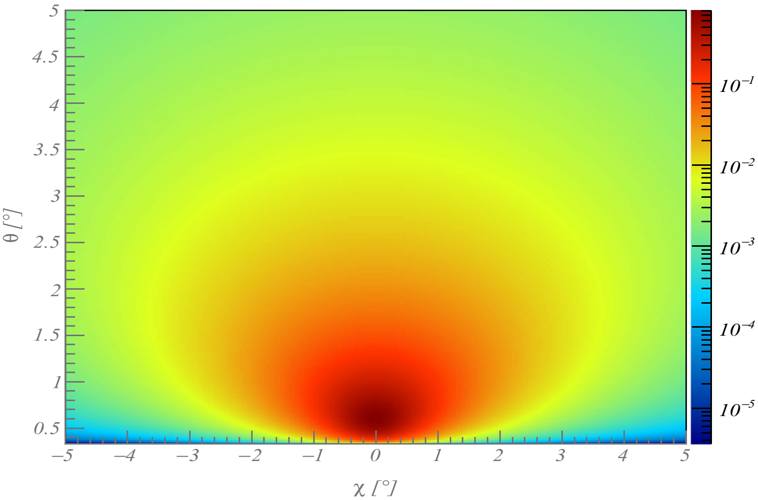


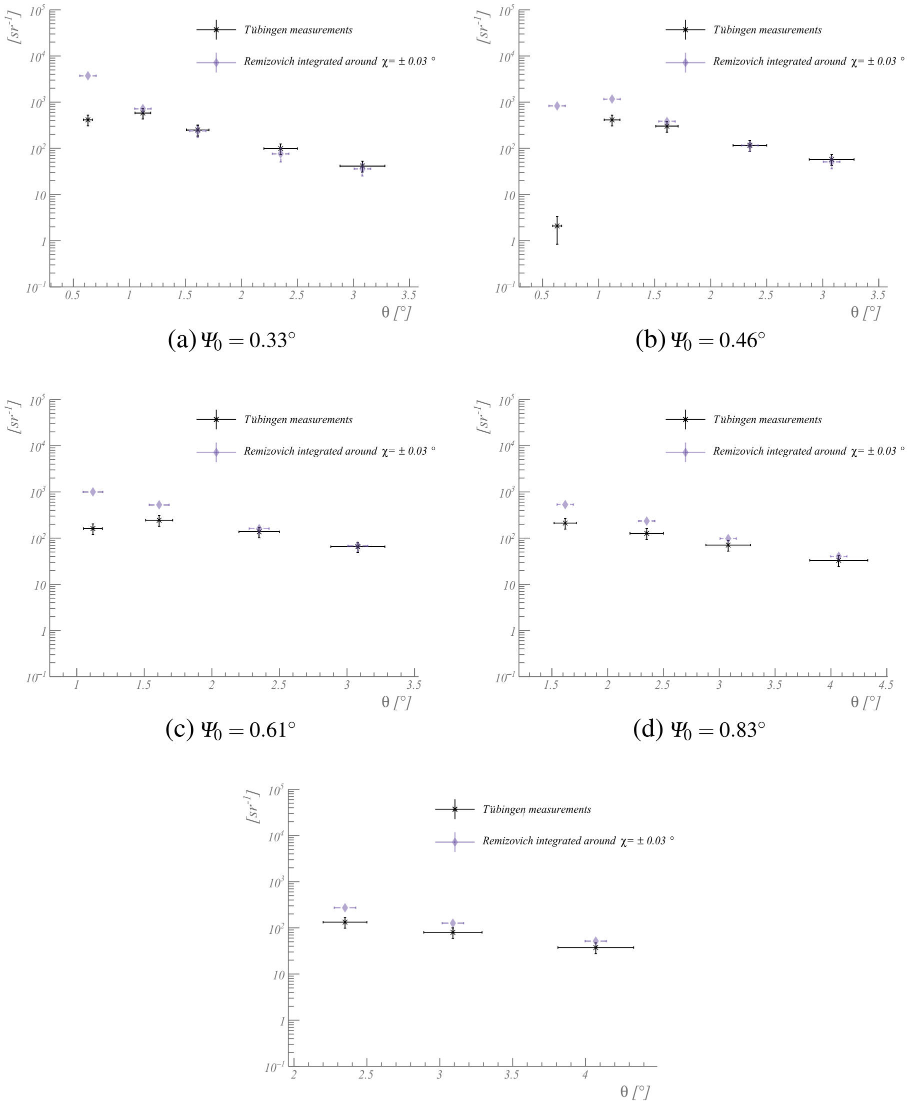
Fig. 2 The two dimensional distribution $\mathscr{R}(\theta, \chi)$ for the case $\Psi_0 = 0.33°$

– There are no energy losses in this process. However, if the ionization-losses process is activated, these may be included. In the case of the Tübingen measurements a gaussian energy loss can be activated. The values for the mean energy loss are taken from the measurements.
– For the Firsov and Remizovich theoretical models there is, by definition, no dependence on the material or the particle energy. On the other hand, in the Tübingen model there is a subtle dependence with the particle's energy.

3.1 Example application and results

We wrote a GEANT4 application to simulate our scattering setup at the Tübingen test facility to cross-check the implementation. The geometry and the definition of our angles is sketched in Fig. 4. This convention follows the one published in [2]. We even included a collimator in the simulation to reproduce precisely the experimental setup. However, in this sample application we were not constrained to measure the scattering only at $\pm 0.03°$ around the beam axis, hence we could probe the whole solid angle range. Besides this fact, most of the experimental characteristics were properly reproduced in our sample application. The incident beam's characteristics (energy, particles' angular distribution, beam diameter, etc.) are taken from the experimental setup [2]. For more details on the actual experimental setup the reader is kindly referred to the cited article.

As a target we used a nickel substrate 6 cm $\times$ 12 cm. With a thickness of 250 μm, coated by a 50 nm gold layer. We deactivated all other processes, leaving *G4GrazingAngleScattering* as the only active process. This way we could isolate any unexpected behaviour of the simulations (i.e. the standard multiple scattering



(a) $\Psi_0 = 0.33°$

(b) $\Psi_0 = 0.46°$

(c) $\Psi_0 = 0.61°$

(d) $\Psi_0 = 0.83°$

(e) $\Psi_0 = 1.03°$

Fig. 3 The scattering efficiency along the polar angle for different incident angles. The *asterisks* correspond to the measurements presented in [2]. The *diamonds* correspond to the predicted value from the Remizovich elastic model (3). This value is calculated integrating around the solid angle seen by the detector (i.e. $d\Omega = 1.3\ \mu$sr). In all cases the energy was 1 MeV

included in GEANT4). We show in Fig. 5 an example of the results of using the *G4GrazingAngleScattering* physical process in this application example. For this example, the tilting angle was $\Psi_0 = 1.03°$ and the scattering model was the one

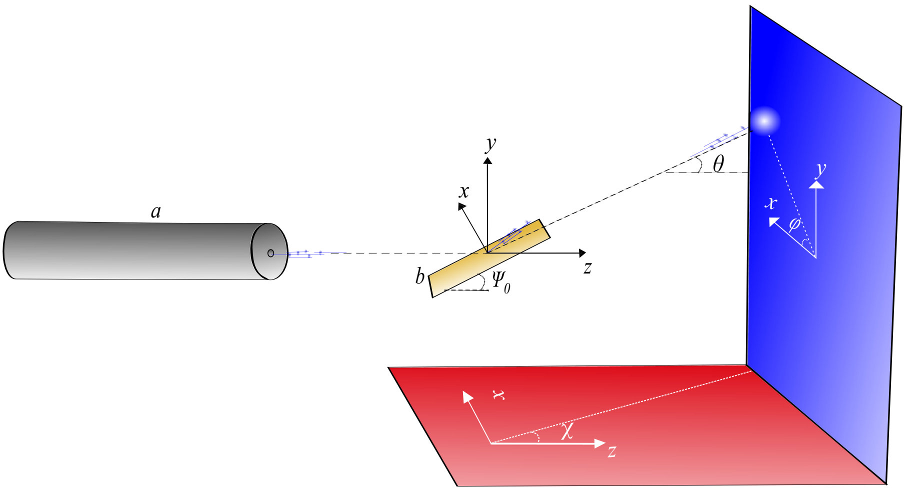


Fig. 4 The geometrical system of reference used in our simulation study. The collimator is labeled "**a**" and the gold-coated nickel target is labeled "**b**". The angles φ and θ coincide with the standard definitions for spherical coordinates. The angle χ is shown in the red plane (parallel to the *xz*-plane). Also shown is the incidence angle Ψ_0, which is controlled by rotating the target along the *x*-axis

based on the Tübingen measurements. The biggest difference between measured and theoretical values appear at the lowest scattering angles (see Fig. 3). However, our process does a compromise when doing the MC simulation. It automatically selects the proper scattering values to either follow the interpolation of the data or, in case the scattering angle is out of the range of the experimental data, to follow one of the models. The results can be seen in the left part of Fig. 5, where the scattering efficiency is simulated in a range where there were no measurements available for this energy-angle combination.

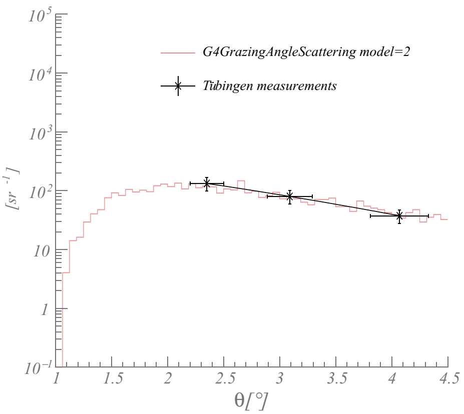


Fig. 5 The scattering efficiency simulated using *G4GrazingAngleScattering* in the sample application mentioned in the text. For this example $\Psi_0 = 1.03°$ and $E_0 = 1$ MeV, and the model used was the Tübingen measurements. The plotted data is restricted to particles with $\chi = \pm 0.03°$

4 Conclusions

We presented an overview of the implementation in GEANT4 of a new class that enables reliable simulations of proton scattering at grazing incidence, based on the Remizovich's theory and/or the interpolation of laboratory measurements taken at the Tübingen accelerator facility. This GEANT4 class, named *G4GrazingAngleScattering*, is a new *VDiscreteProcess* which follows the object-oriented approach of GEANT4. This makes our class suitable to be used in different GEANT4 applications by simply adding it to the list of processes. Therefore, the software tool herein presented can be used in more elaborated simulations where the scattering of soft protons at grazing angles is investigated. Particularly for the forthcoming X-ray observatories that are designed with Wolter-type optics. GEANT4 applications already developed for this purpose, only need to include this process into the simulation to include its effects. Hence, there is no need to develop a dedicate application or physical process to asses the funneling of soft protons through such telescopes, based on experimental data. For completeness we included some theoretical models, but it is not within the scope of this article or the software hereby developed to validate said models. We merely present an addition to the advanced GEANT4 toolkit, that enables the native usage of recent experimental data.

The implementation of laboratory measurements is foreseen to be expanded when new measurements are available. Measurements done at off-axis positions can be easily included to make our class treat azimuthal and zenithal angles in the same manner. These improvements depend of course on the realization, in particular, of measurements at azimuthal angles larger than zero, which are currently in preparation. In the future, measurements with non-polished surfaces like silicon-pore optics may also become available. These can be added as a new model available for the same class. Therefore increasing the versatility of the work here presented. Nevertheless, the general software architecture has been set up and tested and can be easily updated in the future by adding the new experimental data. Upon request, the code can be made available to interested users.

Acknowledgements The AHEAD project (grant agreement n. 654215) which is part of the EU-H2020 programm is acknowledged for partial support.

The research leading to these results has received funding from the European Union's Horizon 2020 Programme under the AHEAD project (grant agreement n. 654215). This work was partially supported by the Bundesministerium für Wirtschaft und Energie through the Deutsche Zentrum für Luft- und Raumfahrt e.V. (DLR) under the grant 50QR0702.

References

1. Allison, J., et al.: Recent developments in Geant4. Nucl. Instrum. Methods Phys. Res. Sect. A **835**, 186–225 (2016)
2. Diebold, S., Tenzer, C., Perinati, E., Santangelo, A., Freyberg, M., Friedrich, P., Jochum, J.: Soft proton scattering efficiency measurements on X-ray mirror shells. Exp. Astron. **39**(2), 343–365 (2015)
3. Fioretti, V., Bulgarelli, A., Malaguti, G., Spiga, D., Tiengo, A.: Monte Carlo simulations of soft proton flares: testing the physics with XMM-Newtonof soft proton flares: testing the physics with

XMM-Newton. In: Proceedings of the SPIE 9905, Space Telescopes and Instrumentation 2016: Ultraviolet to Gamma Ray, 99056U (2016)
4. Firsov, O.B.: Reflection of fast ions from a dense medium at glancing angles. Sov. Phys.-Docklady **11**(8), 732–733 (1967)
5. Kendziorra, E., et al.: The effect of low energy protons on the performance of the EPIC pn-CCD detector on XMM-Newton. Proc. SPIE **4140**, 32–41 (2000)
6. Lo, D.H., Srour, J.R.: Modeling of proton-induced CCD degradation in the Chandra X-ray observatory. IEEE Trans. Nucl. Sci. **50**(6), 2018–2023 (2003)
7. Remizovich, V.S., Ryazanov, M.I., Tilinin, I.S.: Energy and angular distributions of particles reflected in glancing incidence of a beam of ions on the surface of a material. Zh. Eksp. Teor. Fiz. **79**, 448–458 (1980)