Low energy proton scattering at glancing angles: new physics implementation and general validation

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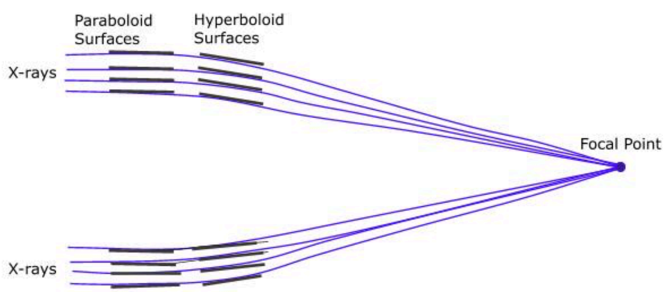
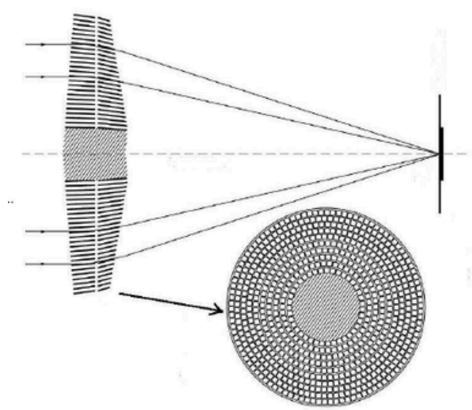
Introduction - 1

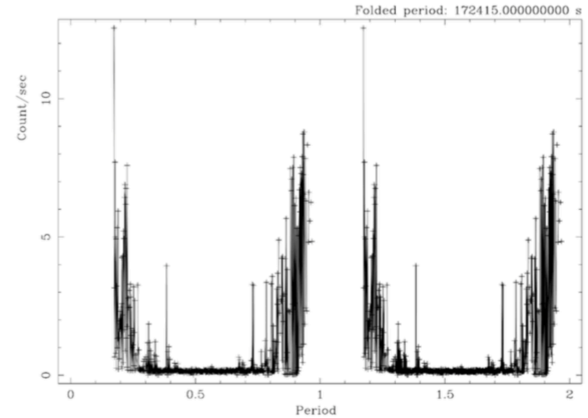
- X-ray focusing telescopes use Wolter type-1 X-ray optics for grazing angle reflection
- As discovered after the launch in 1999 of NASA/Chandra and ESA/XMM-Newton telescopes, <u>low energy protons (< 300 keV, so-called "soft"protons) can enter the field of view, scatter at small angles and reach the focal plane</u>
- Soft protons decreased Chandra/ACIS F-I CCD CTE and cause intense backgroud flares on XMM-Newton/EPIC detectors
- What to expect for the ESA/ATHENA future X-ray observatory?



X-ray shells
(e.g. XMM-Newton)

Silicon Pore Optics
(ATHENA)





XMM-Newton soft proton flares (Fioretti+2016)

Introduction - 2

Current issues:

- we still don't know the physics behind soft proton scattering
- models for the input proton popolation poor or inexistent

Our goals

1. Implementation of the Firsov and Remizovich (no energy losses approximation) scattering on top of Geant4 10.2

2. Geant4 soft proton physics verification

3. Geant4 soft proton physics validation: comparison with experimental data

This activity is part of the ESA/AREMBES (Athena Radiation Environment Models and X–ray background Effects Simulator) project (The ESA Contract No. 4000116655/16/NL/BW is acknowledged) – see Lotti's talk on Monday

All results in V. Fioretti et al., "Geant4 simulations of soft proton scattering in X-ray optics: a tentative validation using laboratory measurements", submitted to Exp. Astr.

Grazing angle proton scattering in Geant4 – current status

Coulomb scattering (single and multiple) is the only available process in Geant4 to describe grazing angle proton reflections

- Coulomb multiple scattering:
  - first used by Nartallo+2001 to evaluate the impact of soft protons on XMM-Newton mission using Geant4 simulations.
- Firsov model (azimuthal integration of the Remizovich elastic model):
  - it is implemented in Geant4 (<9.1) by Lei+2004
  - used in XMM-Newton simulations
  - Firsov model increases the efficiency of low angle proton scatterings at small angles and the related proton flux on the focal plane.
  - <u>Firsov model was not implemented in the official release</u>.

Grazing angle proton scattering in Geant4 – new implementation

AREMBES/WP3.3 goal:

- implementation of the Firsov and Remizovich models on top of Geant4 10.2;
- comparing both built-in Geant4 models and new models with laboratory measurements.

The following Geant4 built-in models are compared:

- Multiple Coulomb scattering, provided by the Option 3 and Option 4 EM physics lists (**MSC_opt3 and MSC_opt4**);
- Single Coulomb scattering, provided by the G4EmStandardPhysicsSS EM physics list (**SS**).

Simulation set-up

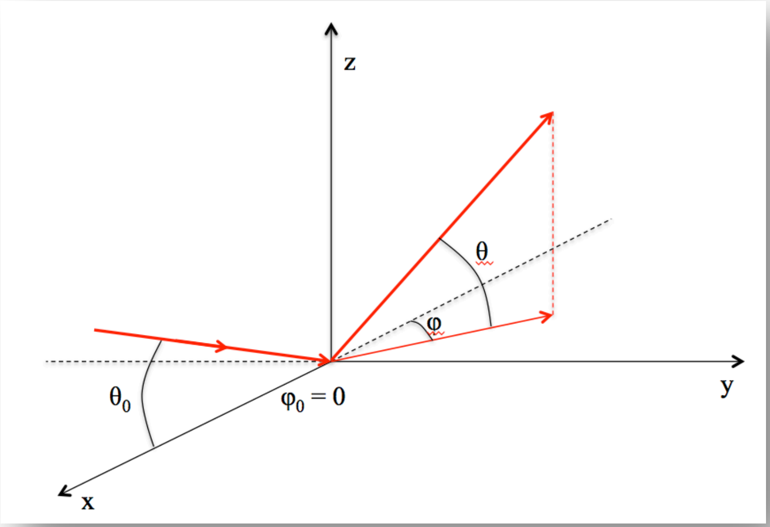
- Geant4 release: 10.2
- Simulation framework: BoGEMMS
  - the user can set at run-time the proton energy and incident angle range where to apply the new models.
  - Models can also be combined and used in the same simulation using different energy or incident angle ranges.

- The X-ray mirror geometry is approximated by a slab based on eRosita configuration:
  - Ni slab (10x10 cm), 270 μm thick – bottom
  - Au slab (10x10 cm), 50 nm thick - top

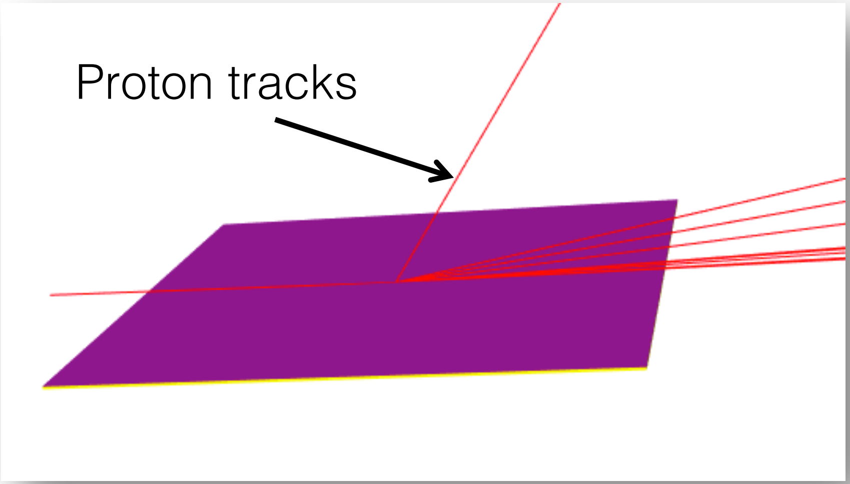
- Physics:
- cross section of Firsov and Remizovich is assumed to be 1
- no dependence has been currently inserted on the reflecting material.

Simulation set-up

Angular system of reference



Geometry set-up



Remizovich (elastic) model implementation

The Remizovich model (*Remizovich+1980*) describes particles reflected by solids at glancing angles (< 1 deg.) in terms of the Boltzmann transport equation using the diffuse approximation and the model of continuous slowing down in energy, in the case of small angle collisions.

In the elastic scattering approximation gives the probability W of proton reflection over the polar angle θ and the azimuthal angle φ as:

$$\mathrm{W}_{\mathrm{el}}(\Psi,\chi) = \frac{1}{12\pi^2\Psi^{1/2}}\left[\frac{\omega^4}{1+\omega^2} + \omega^3\arctan(\omega)\right],$$

$$\omega = \left\{\frac{3\Psi}{\Psi^2 - \Psi + 1 + (\chi/2)^2}\right\}^{1/2}.$$

$$\Psi = \theta/\theta_0,\ \chi = \phi/\theta_0$$

Firsov model implementation

- The Firsov model (Firsov, 1967) is the azimuthal integration of the Remizovich elastic approximation. It describes the probability W of proton reflection over the polar angle θ while integrating over the azimuthal angle **φ.**
- In the Geant4 implementation, following the original Geant4 implementation by F. Lei, the azimuth angle is assumed to be 0 (forward scattering).

$$\mathrm{W}(\Psi) = \frac{3}{2\pi}\frac{\Psi^{3/2}}{1+\Psi^3}.$$

$$\Psi = \theta/\theta_0,$$

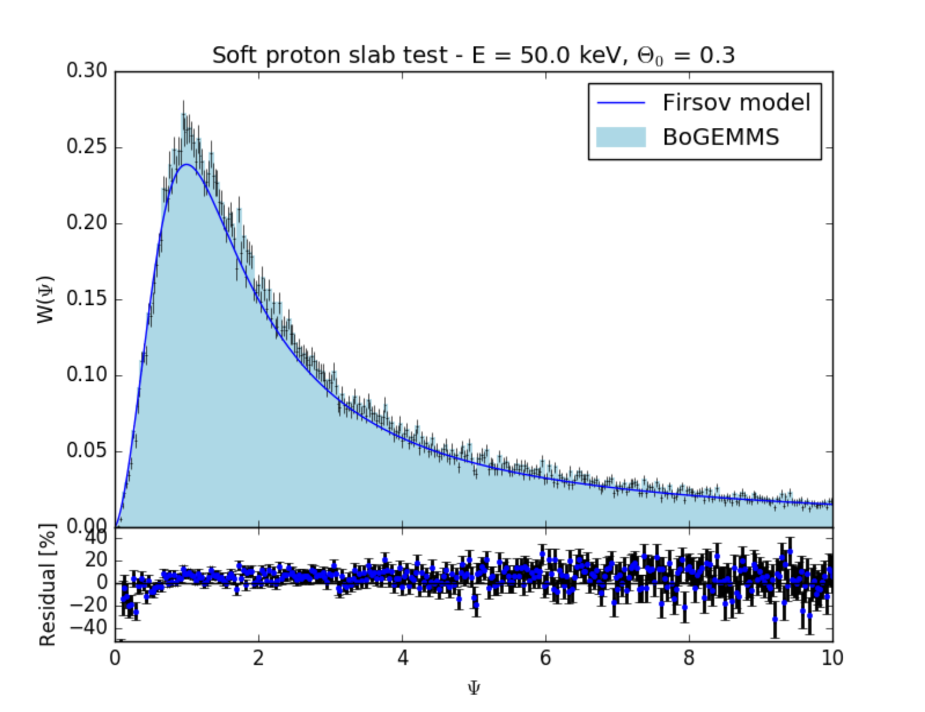
SS and MSC Geant4 implementation

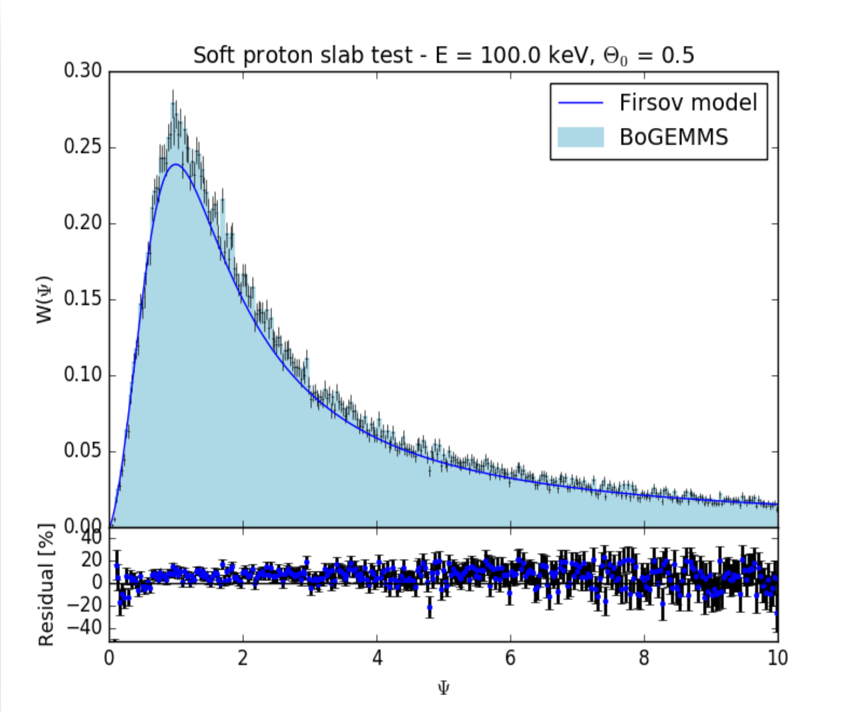
In the single or multiple Coulomb scattering, when a charged particle traverses a medium, it undergoes one or more scatterings due to Coulomb interactions with the electron field of the nuclei, as described by the Rutherford cross section.

We use the following Geant4 electromagnetic physics lists:

- emstandard_opt3: Urban model of multiple scattering (G4UrbanMscModel)
- emstandard_opt4: a combination of multiple scattering G4WentzelVIMscModel and single scattering model G4eCoulombScatteringModel.
- G4EmStandardPhysicsSS: only the single scattering model is defined, for any scattering angle.

Firsov: Simulation vs Model

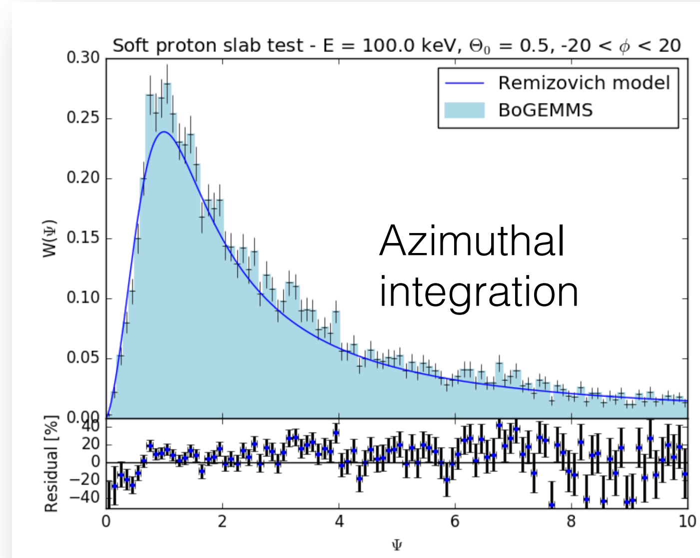


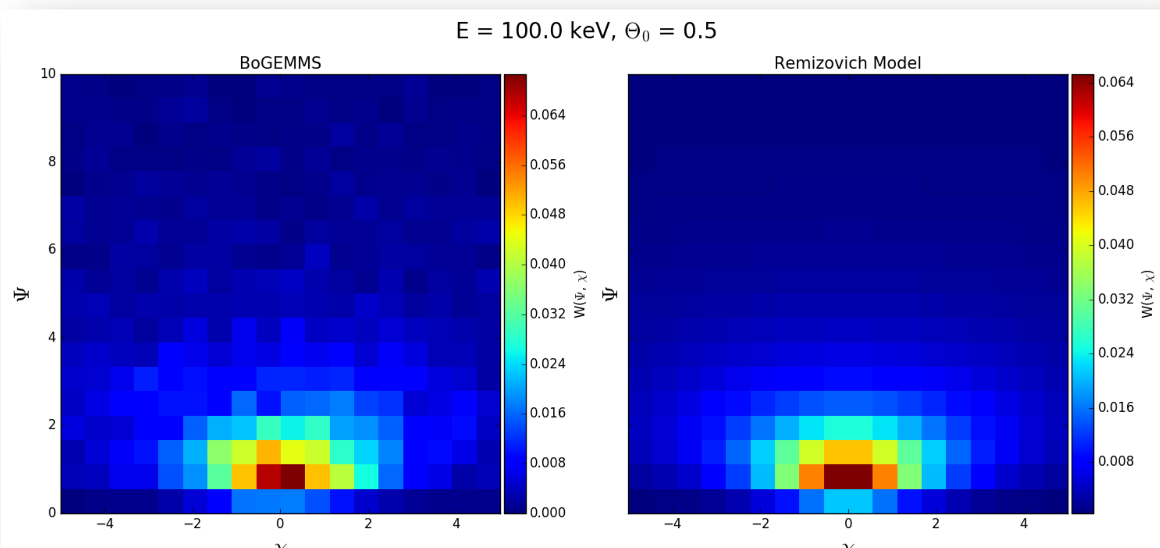


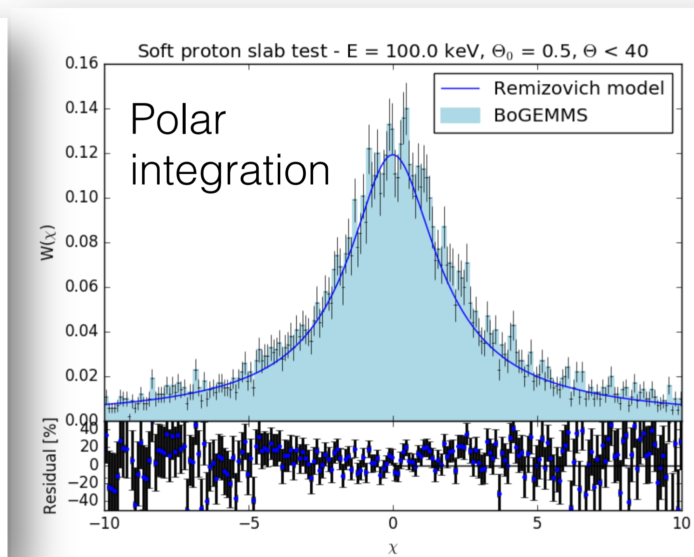
We are able to reproduce the Firsov distribution (at ϕ=0) within an uncertainty of +/-10% wrt the analytical values.

Remizovich (elastic): Simulation vs Model

We are able to reproduce the Remizovich distribution within +/-20% wrt the analytical values.







Remizovich (elastic) model: benchmarks and optimization

- The probability distribution is computed at run time for each particle
- This approach is feasible for Firsov (one free parameter - θ) but not for the Remizovich distribution (two free parameters – ϑ and ϕ - and complex algorithm):

Simulation CPU time for all the tested models in units of time required by multiple scattering (emstandard_option3). The performance test refers to a run of 10^4 protons at 250 keV for an incident angle of 0.36 degrees.

	MSC-opt3	MSC-opt4	SS	Remizovich	Firsov
CPU time	1	1.05	21.25	366.7	3.1

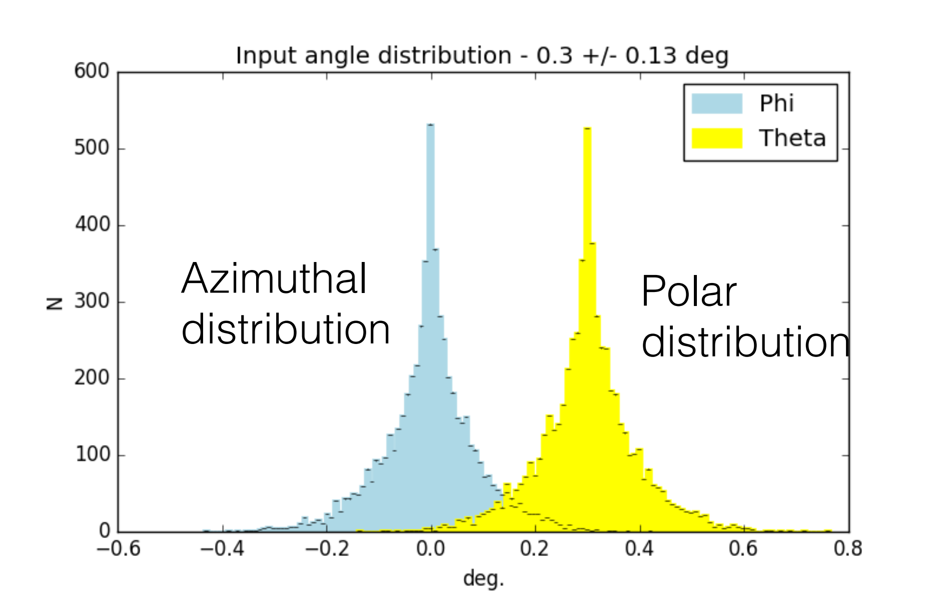
Proposed optimization solutions:

✓ **algorithm optimization: DONE (50% CPU time)**
✓ **probability distribution binning fine tuning: DONE**
x parallelization of the for loop (e.g. openMP): to be tested
x Geant4 multithreading: to do
x tabulated angle distribution: to be tested

Laboratory measurements of soft proton scattering

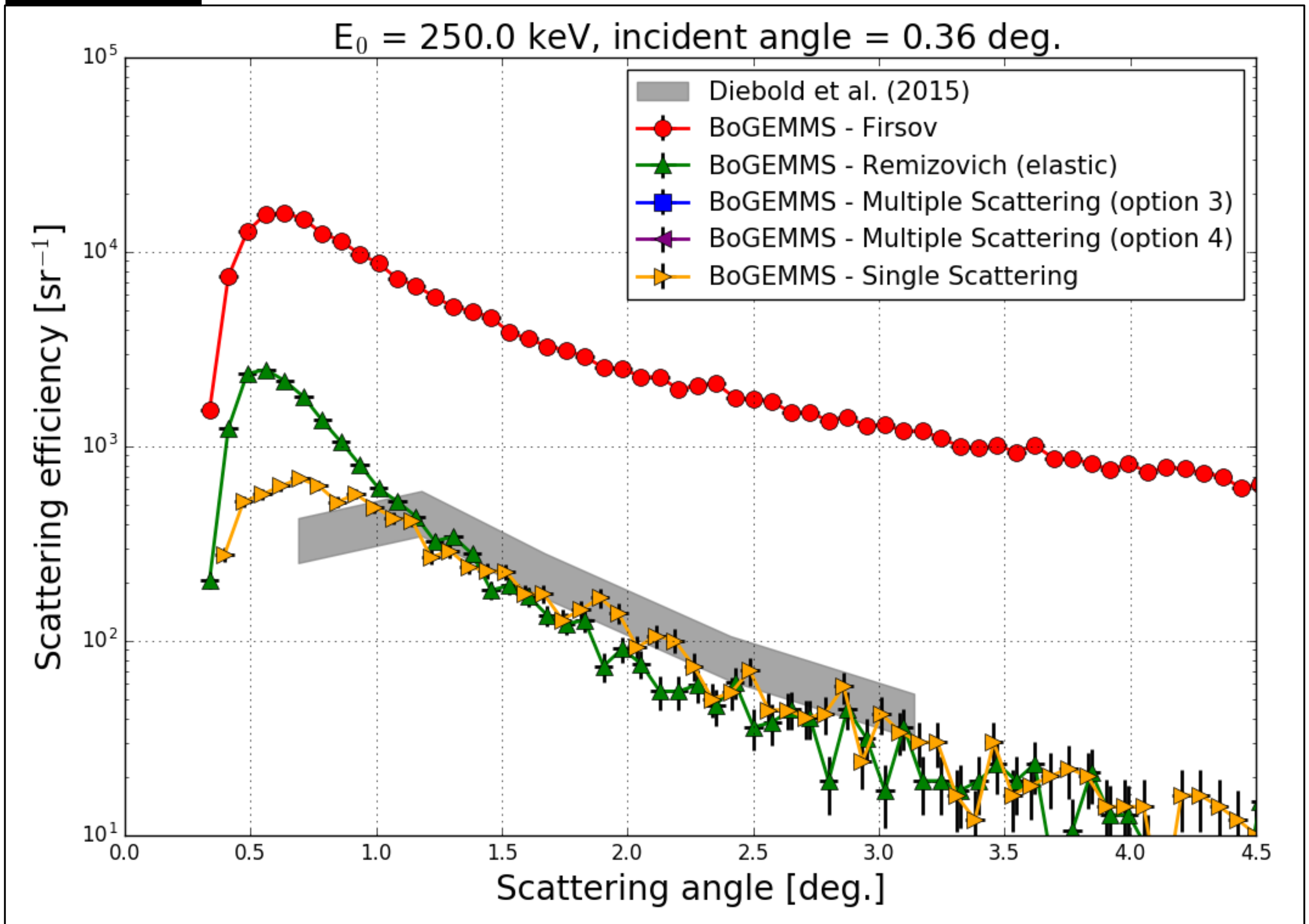
- The experiment of Diebold+2015 evaluates the scattering efficiency, in sr^{-1}, and the energy loss of protons at 250, 500, and 1000 keV interacting with eRosita shell samples at glancing angles in the 0.3 – 1.2 deg. range.

- The uncertainty in the incident proton angle is simulated using as proton source a beam profile with a standard deviation equal to the angle error, as shown in Figure 6.

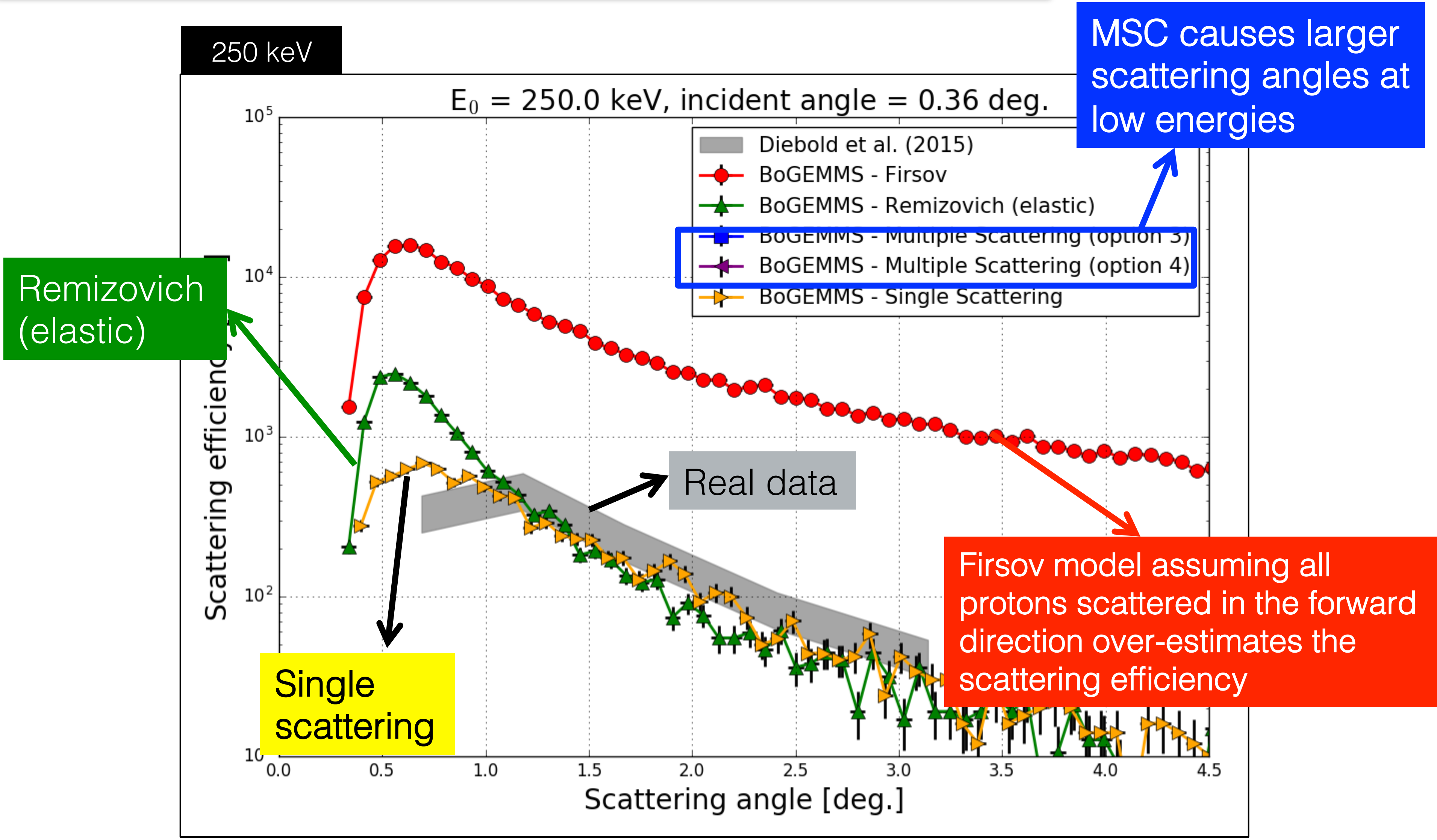


Comparison with real data – Scattering efficiency

250 keV



Comparison with real data – Scattering efficiency

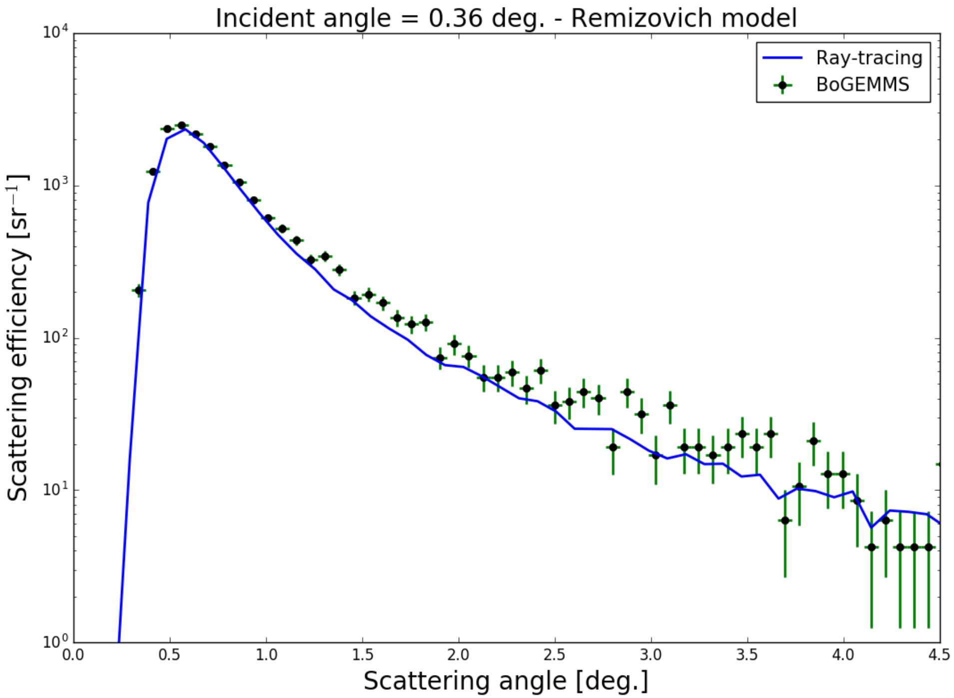


Remizovich (elastic): Geant4 vs Ray-Tracing

An independent ray-tracing simulation of the Remizovich elastic model has also been developed as part of AREMBES activities

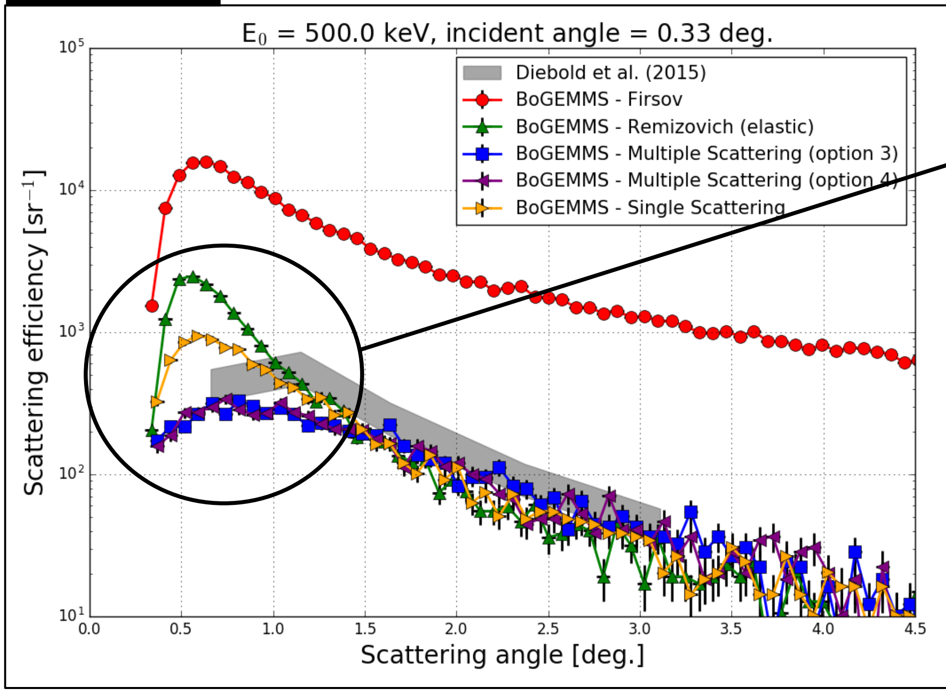
The two simulations are consistent (ray-tracing data courtesy of T. Mineo)

Scattering efficiency



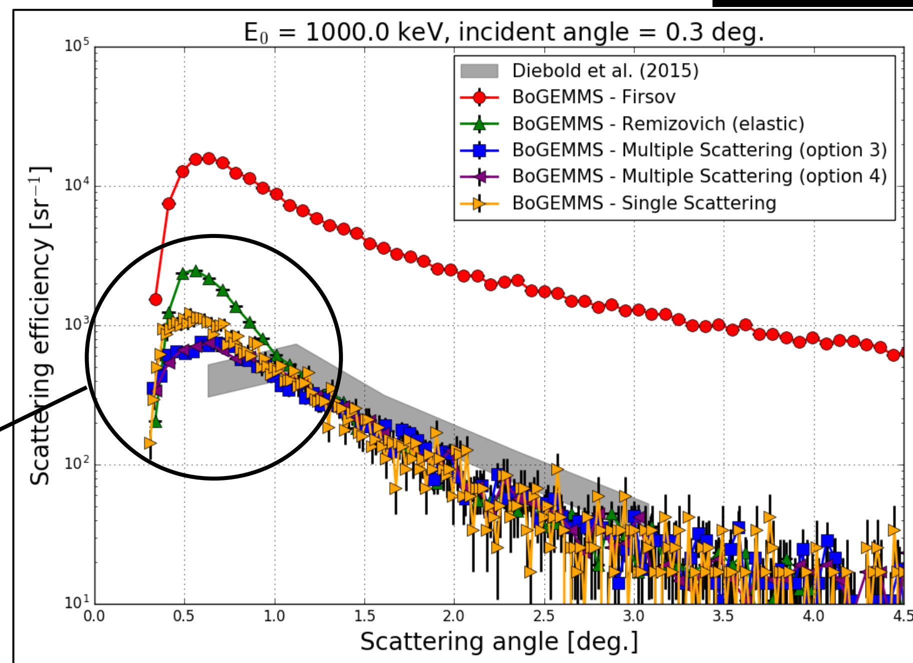
Comparison with real data – Scattering efficiency

500 keV



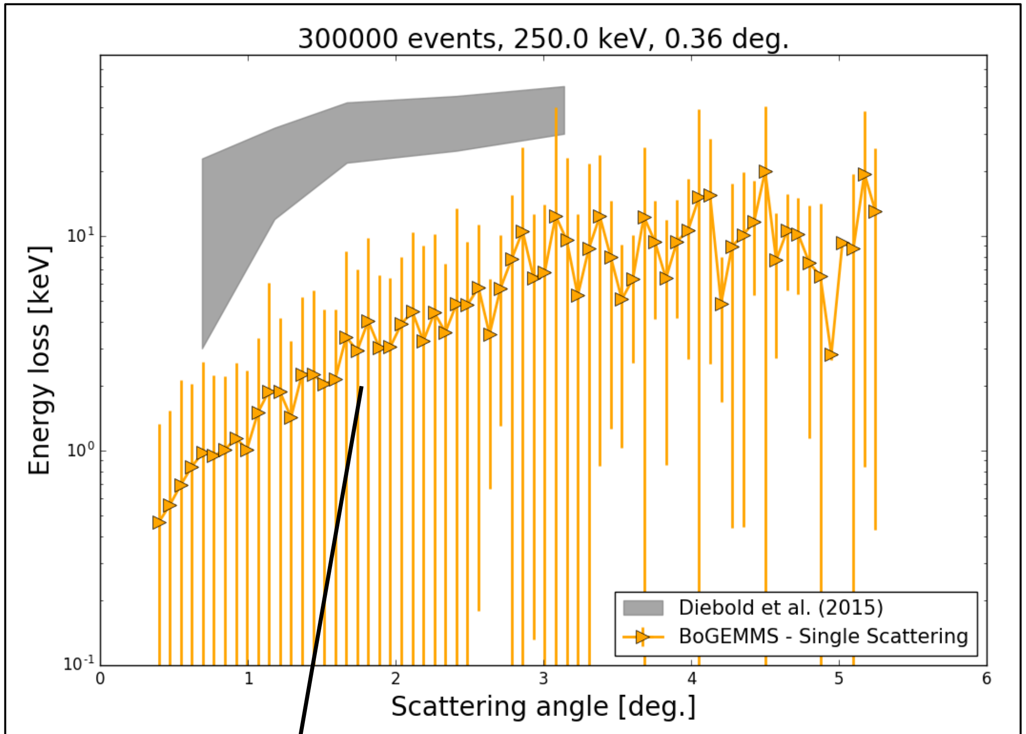
- Remizovich and SS models predict higher efficiencies at low scattering angles, contrary to the MSC models.
- At large scattering angles all models are consistent with the experimental data (no difference is found between option3 and option4)

1 MeV



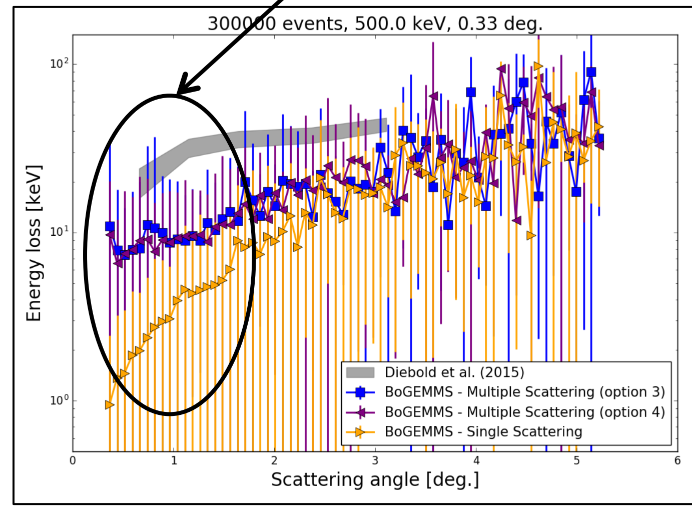
- SS and MSC give close results for 1 MeV protons
- Remizovich still gives higher results

Comparison with real data – Energy losses

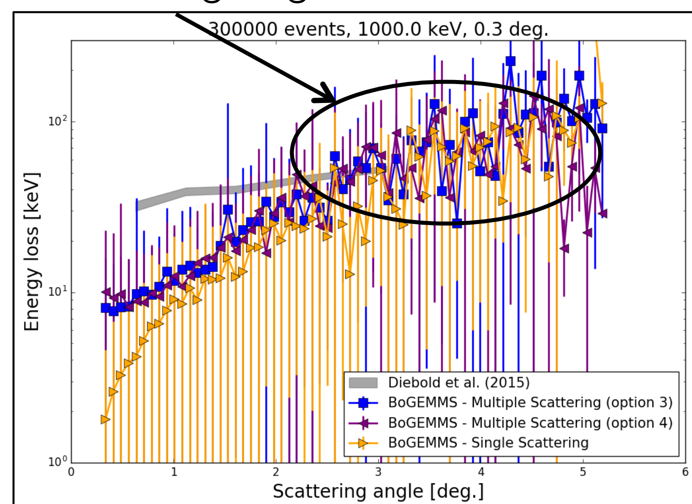


At low energy and incident angles, SS gives energy losses less than 1 keV at the specular reflection angles, and up to ≈10 keV for larger scattering angles, about 10 times less than the experimental data.

MSC energy losses close to the experimental one at low angles



MSC and SS consistent at large scattering angles



A model for grazing angles soft proton scattering

- we can discard multiple scattering as the model able to reproduce soft proton funnelling
- we can affirm that Coulomb single scattering can represent, until further measurements at lower energies, the best approximation for the proton scattered angular distribution at the exit of X-ray optics.

BUT

Experimental data are not completely representative of the soft proton scattering experienced by current X-ray telescopes, because of

- the lack of efficiency measurements at low energies (<250 keV)
- the lack of small reflection angles

For these reasons, it is not yet possible to advertise any of the tested models as a very good approximation for the simulation of the most accurate one for the simulation of the scattering of low energy protons experienced by ATHENA X-ray optics.

Geant4 Remizovich implementation

The Remizovich model in its approximated form has proven a general consistency with the measurements, and the present Remizovich Geant4 implementation:

- is currently being used as basis for the development for an implementation of the Remizovich effect to be proposed for the December Geant4 toolkit release (activity carried in collaboration with the Geant4 LowEnergy working group)

- Inclusion in the *Space Physics list* of the AREMBES project (see Dondero's talk) will be possible to the user's choice.

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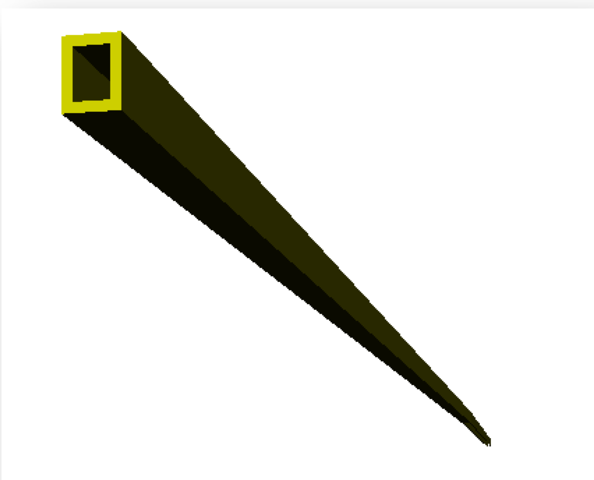
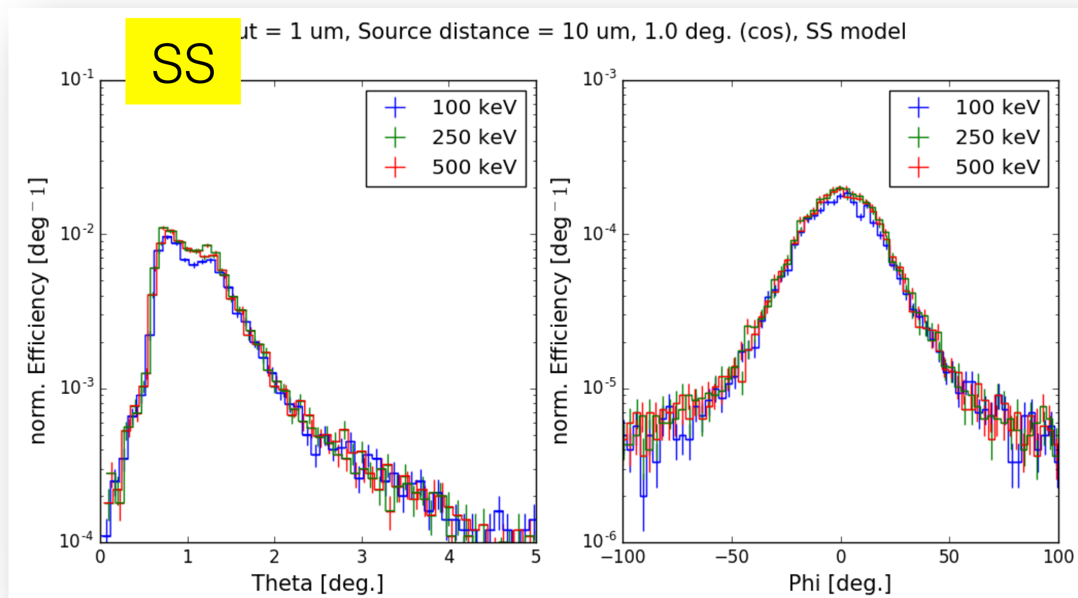
ATHENA soft proton induced background

1. Remizovich Geant4 implementation already provided to ESA

2. Both Remizovich and SS models currently used in AREMBES simulation of soft proton interaction with ATHENA/SPO (tight collaboration and cross-check with ESA people)

First results from one Silicon pore





ATHENA soft proton induced background

1. Remizovich Geant4 implementation already provided to ESA

2. Both Remizovich and SS models currently used in AREMBES simulatio n of soft proton interaction with ATHENA/SPO (tight collaboration and cross-check with ESA people)

3. AREMBES can contribute on the magnetic diverter specifications in terms, e.g., of energy and angular distribution, and intensity of the protons emerging from the SPO

3. A magnetic diverter will implemented as part of the AREMBES activities as “exploratory” investigation (complex geometry, running time vs simul ation accuracy)

A model for grazing angles soft proton scattering - Summary

- if we consider the proton distribution at 250 keV, Remizovich and single scattering are well consistent with the experimental scattering efficiency except for very small, < 1 deg., scattering angles, where higher efficiencies are found in the simulation;

- the single scattering induced scattering efficiency at small angles is the closest to the observation, but the energy losses are a factor 10 less than the experimental ones;

- multiple scattering results in the larger energy losses, close to the laboratory measurements, for energies in the 500-1000 keV range;

- at large incident and consecutively scattering angles, the angular distribution does not depend on the primary proton energy and all the models give similar results;

- no differences are found between the EM opt3 and opt4 list multiple scattering settings.

Back-up slides

Experimental data of reference

The experiment of Diebold+2015 evaluates the scattering efficiency, in sr^{-1}, and the energy loss of protons at **250, 500, and 1000 keV** interacting with eRosita shell samples at glancing angles in the **0.3 – 1.2 deg**. range.

The general set-up consists of a proton beam line produced by a ion accelerator facility hitting the X-ray mirror shell sample at different angles and then collected by a shiftable proton detector:

- the incident angle has a precision, in terms of tilt angle, of 0.006 deg.;
- the eRosita target shell is composed by a Nickel substrate of 270 μm coated by 50 nm of Gold and different sample sizes, ranging from a length of 10 cm to 12 cm, were used with no impact on the measurements;
- the proton detector consists of a 8 mm wide Silicon surf barrier detector characterized by a detection efficiency of almost 100% and an overall accuracy within ±10 keV.