Low Energy Electromagnetic Physics

Maria Grazia Pia
INFN Genova
Maria.Grazia.Pia@cern.ch
on behalf of the Low Energy Electromagnetic Working Group

http://www.ge.infn.it/geant4/lowE/

What is

- A package in the Geant4 electromagnetic package
  - *geant4/source/processes/electromagnetic/lowenergy/*
- A set of processes extending the coverage of electromagnetic interactions in Geant4 down to "*low*" energy
  - 250 eV *(in principle even below this limit)/100* eV for electrons and photons
  - down to the approximately the ionisation potential of the interacting material for hadrons and ions
- A set of processes based on detailed models
  - shell structure of the atom
  - precise angular distributions
- Complementary to the "standard" electromagnetic package

Overview of physics

- Compton scattering
- Rayleigh scattering
- Photoelectric effect
- Pair production
- Bremsstrahlung
- Ionisation
- Polarised Compton
- + atomic relaxation
  - fluorescence
  - Auger effect

  following processes leaving a vacancy in an atom

- In progress
  - More precise angular distributions (Rayleigh, photoelectric, Bremsstrahlung etc.)
  - Improved PIXE

in two "flavours" of models:
- based on the Livermore Library
- à la Penelope

- Development plan
  - *Driven by user requirements*
  - *Schedule compatible with available resources*

Software Process

A rigorous approach to software engineering

- in support of a better quality of the software
- especially relevant in the physics domain of Geant4-LowE EM
- several mission-critical applications (space, medical…)

Bsed on the UP

A life-cycle model that is both iterative and incremental

Collaboration-wide Geant4 software process, tailored to the specific projects

Huge effort invested into SPI

- *started from level 1 (CMM)*
- *in very early stages: chaotic, left to heroic improvisation*

current → status

- ***Public URD***
- *Full traceability through UR/OOD/implementation/test*
- *Testing suite and testing process*
- *Public documentation of procedures*
- *Defect analysis and prevention*
- *etc.…*

User requirements

Various methodologies adopted to **capture** URs

- **Elicitation through interviews and surveys**
  - *useful to ensure that UR are complete and there is wide agreement*
- **Joint workshops with user groups**
- **Use cases**
- **Analysis of existing Monte Carlo codes**
- **Study of past and current experiments**
- **Direct requests from users to WG members**

User Requirements

GEANT4 LOW ENERGY ELECTROMAGNETIC PHYSICS

Posted on the WG web site

User Requirements Document

Status: in CVS repository

Version: 2.4
Project: Geant4-LowE
Reference: LowE-URD-V2.4
Created: 22 June 1999
Last modified: 26 March 2001
Prepared by: Petteri Nieminen (ESA) and Maria Grazia Pia (INFN)

LowE processes
based on Livermore Library

Photons and electrons

different approach w.r.t. Geant4 standard e.m. package

- Based on evaluated data libraries from LLNL:
  - EADL *(Evaluated Atomic Data Library)*
  - EEDL *(Evaluated Electrons Data Library)*
  - EPDL97 *(Evaluated Photons Data Library)*

  especially formatted for Geant4 distribution *(courtesy of D. Cullen, LLNL)*

- Validity range: 250 eV - 100 GeV
  - The processes can be used down to 100 eV, with degraded accuracy
  - In principle the validity range of the data libraries extends down to ~10 eV

- Elements Z=1 to Z=100
  - Atomic relaxation: $Z > 5$ *(transition data available in EADL)*

Calculation of cross sections

Interpolation from the data libraries:

$$\log(\sigma(E)) = \frac{\log(\sigma_1)\log(E_2 / E) + \log(\sigma_2)\log(E / E_1)}{\log(E_2 / E_1)}$$

E_1 and E_2 are the lower and higher energy for which data (σ_1 and σ_2) are available

Mean free path for a process, at energy E:

$$\lambda = \frac{1}{\sum_i \sigma_i(E) \cdot n_i}$$

n_i = atomic density of the i^{th} element contributing to the material composition

Polarisation

Cross section:

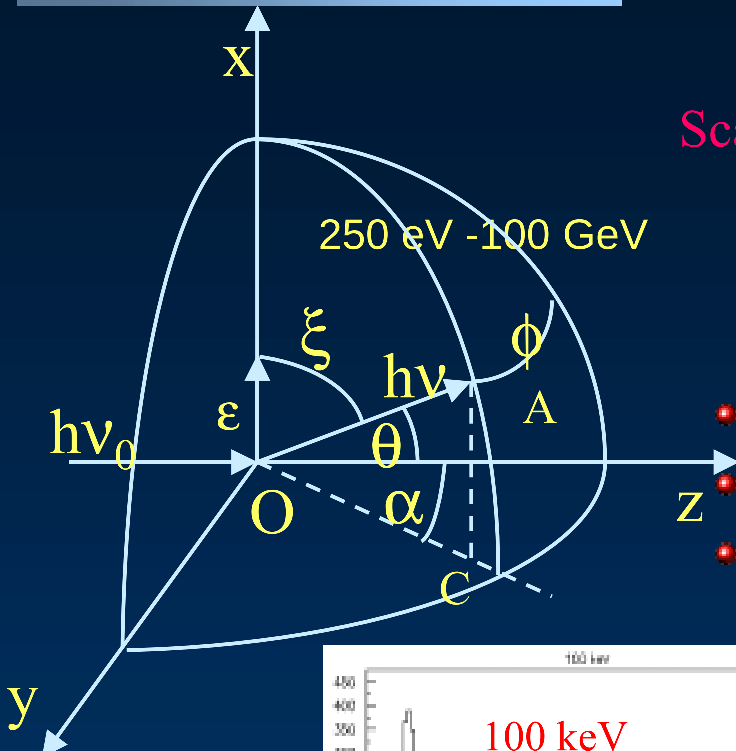
$$\frac{d\sigma}{d\Omega} = \frac{1}{2} r_0^2 \frac{h\nu^2}{h\nu_0^2}\left[\frac{h\nu_0}{h\nu}+\frac{h\nu}{h\nu_0}-2\sin^2\theta\cos^2\phi\right]$$

$$\cos\xi = \sin\theta\cos\phi \quad \Rightarrow \quad \sin\xi = \sqrt{1-\sin^2\theta\cos^2\phi} = N$$

Scattered Photon Polarization

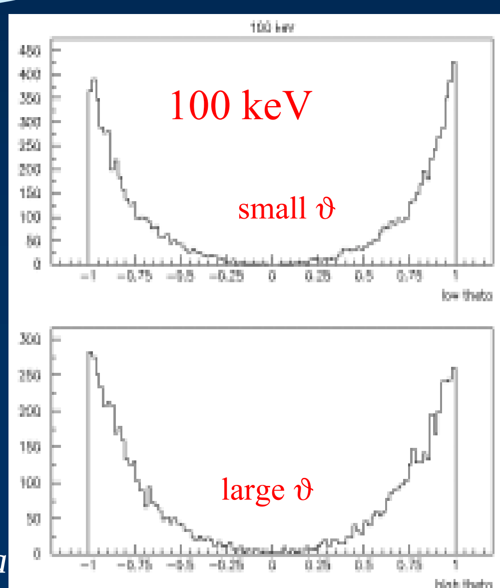
$$\overline{\varepsilon'_\perp} = \frac{1}{N}\left(\cos\theta\,\hat{j} - \sin\theta\sin\phi\,\hat{k}\right)\sin\beta$$

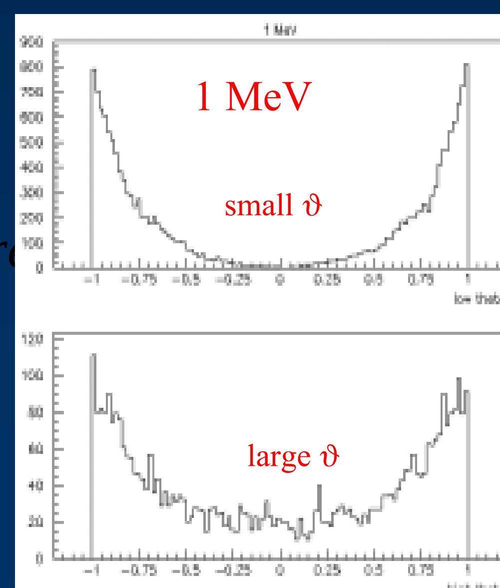
$$\overline{\varepsilon'_\parallel} = \left(N\hat{i} - \frac{1}{N}\sin^2\theta\sin\phi\cos\phi\,\hat{j} - \frac{1}{N}\sin\theta\cos\theta\cos\phi\,\hat{k}\right)\cos\beta$$

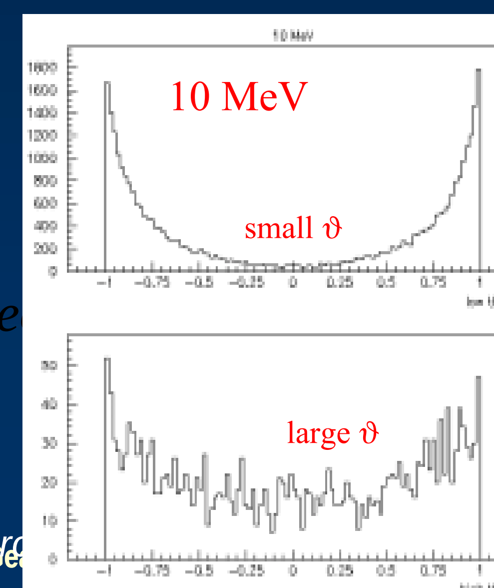


- θ Polar angle
- ϕ Azimuthal angle
- ε Polarization vector

Low Energy Polarised Compton







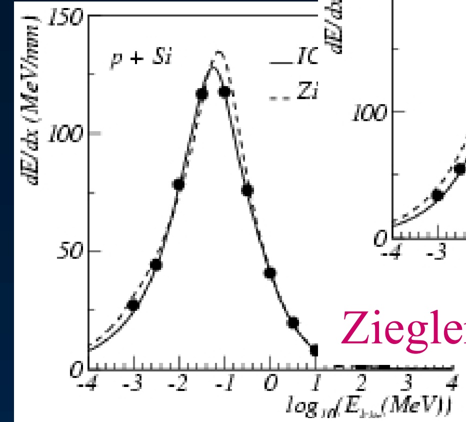
Hadrons and ions

- Variety of models, depending on
  - energy range
  - particle type
  - charge
- Composition of models across the energy range, with different approaches
  - analytical
  - based on data reviews + parameterisations
- Specialised models for fluctuations
- Open to extension and evolution

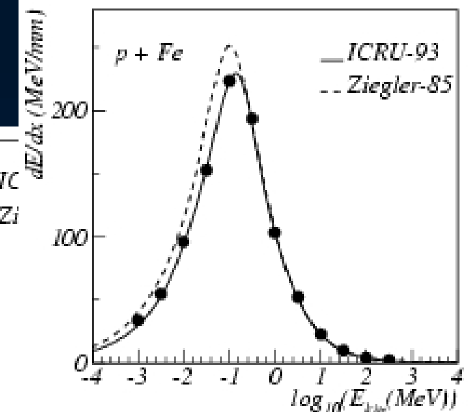
Positive charged hadrons

- Bethe-Bloch model of energy loss, E > 2 MeV
- 5 parameterisation models, E < 2 MeV
  - *based on Ziegler and ICRU reviews*
- 3 models of energy loss fluctuations

- Density correction for high energy
- Shell correction term for intermediate energy



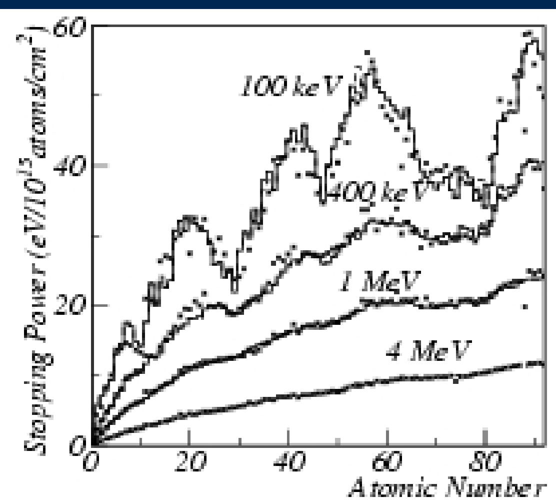
Ziegler and ICRU, Si



Ziegler and ICRU, Fe

-Spin dependent term
- Barkas and Bloch terms

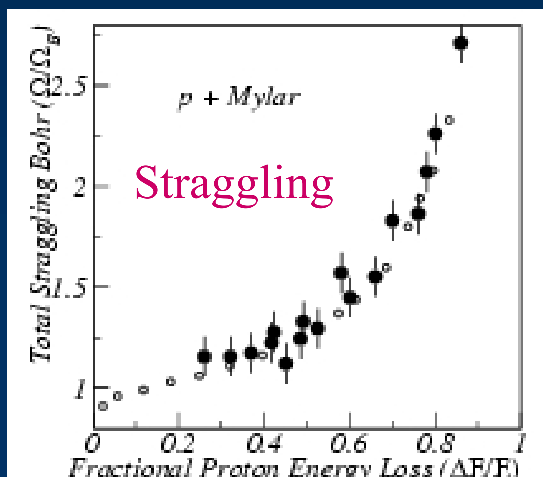
-Chemical effect for compounds
- Nuclear stopping power
- PIXE included <u>*(preliminary)*</u>

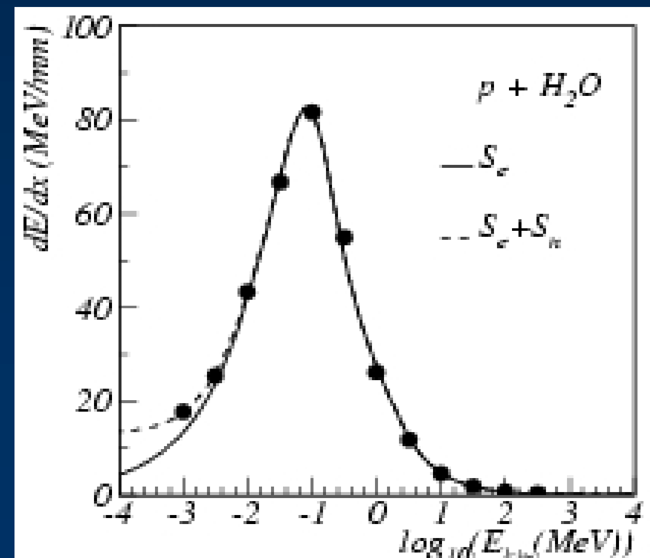


Stopping power

Z dependence for various energies

Ziegler and ICRU models



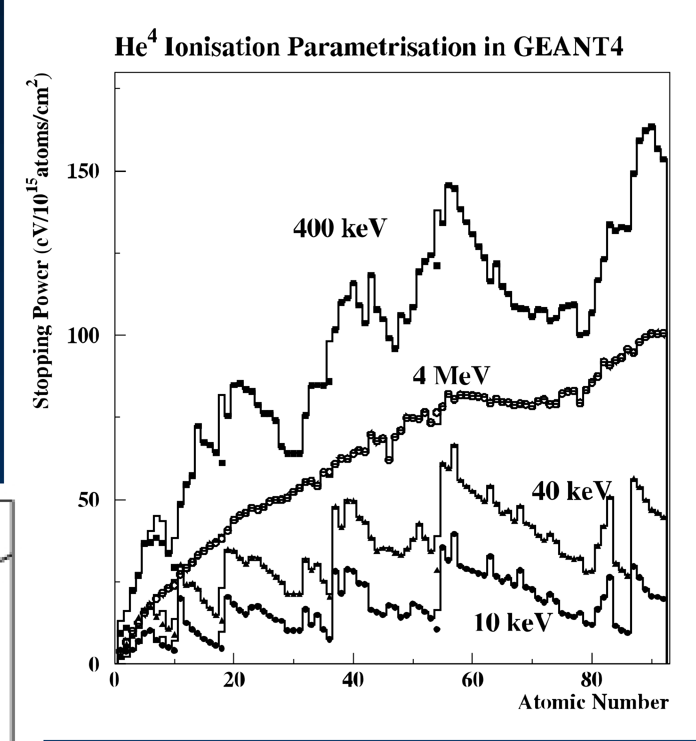


Nuclear stopping power

Positive charged ions

- Scaling: $$S_{ion}(T) = Z_{ion}^2 S_p(T_p),\ T_p = T\frac{m_p}{m_{ion}}$$
- $0.01 < \beta < 0.05$ parameterisations, Bragg peak
  - *based on Ziegler and ICRU reviews*
- $\beta < 0.01$: Free Electron Gas Model

- Effective charge model
- Nuclear stopping power



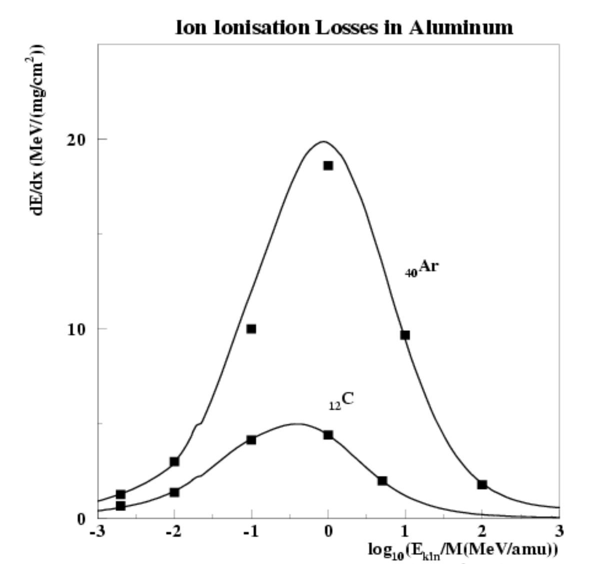
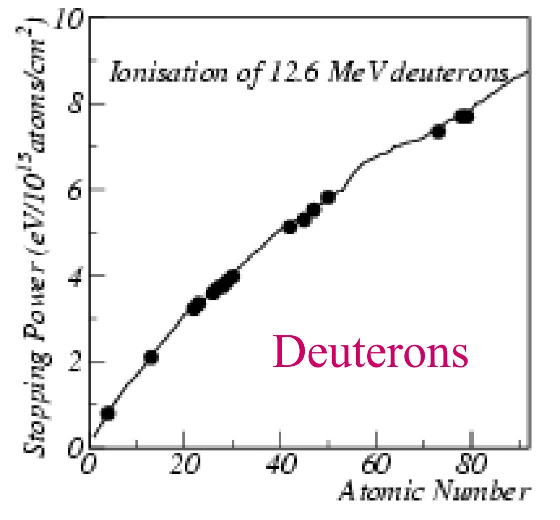
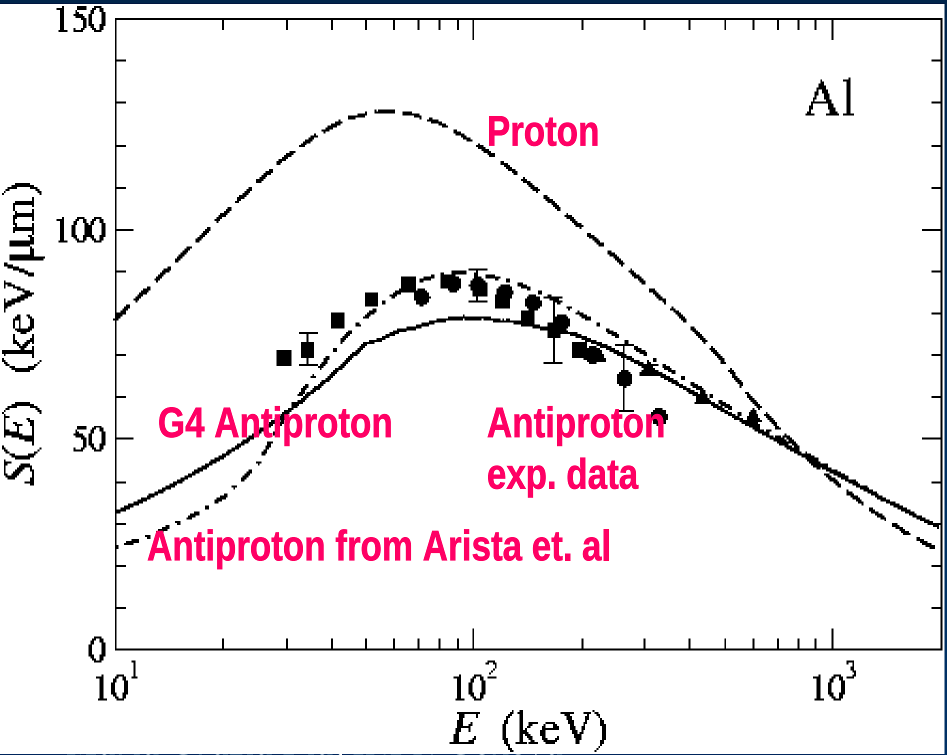


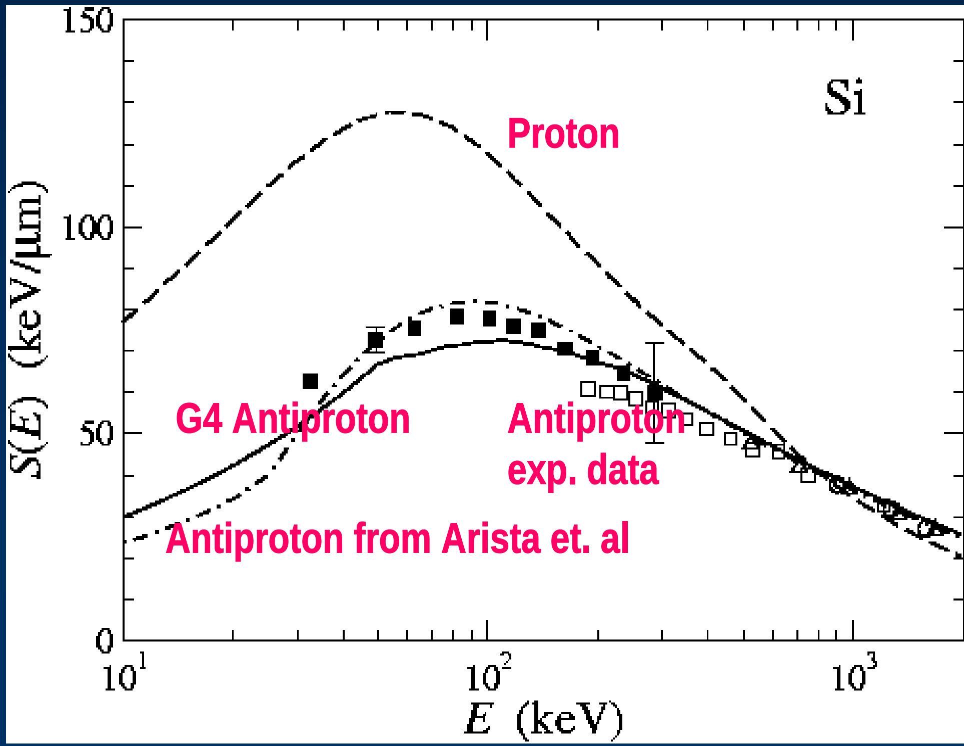
Figure 9: Ion electronic stopping power in aluminum. Points - the best fit on the data from Ref.[12], solid line - GEANT4 parameterisation. The accuracy of the data is about 5 %.



Models for antiprotons

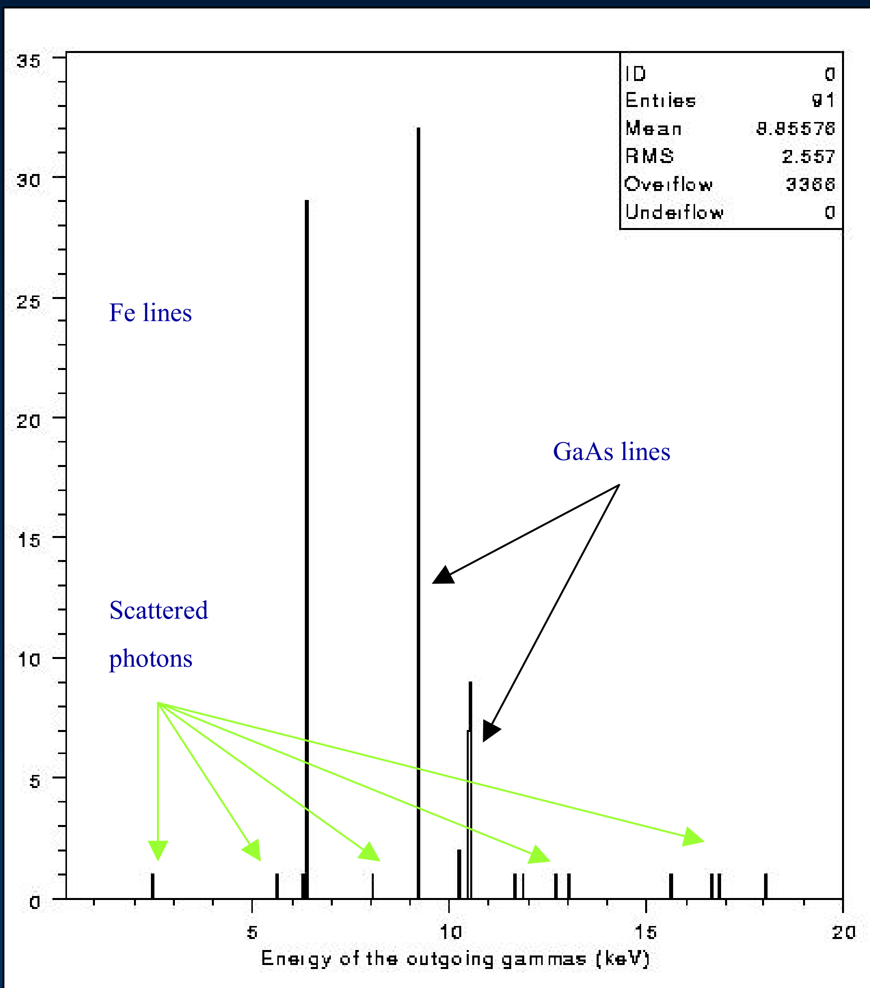
- $\beta > 0.5$ — Bethe-Bloch formula
- $0.01 < \beta < 0.5$ — Quantum harmonic oscillator model
- $\beta < 0.01$ — Free electron gas model



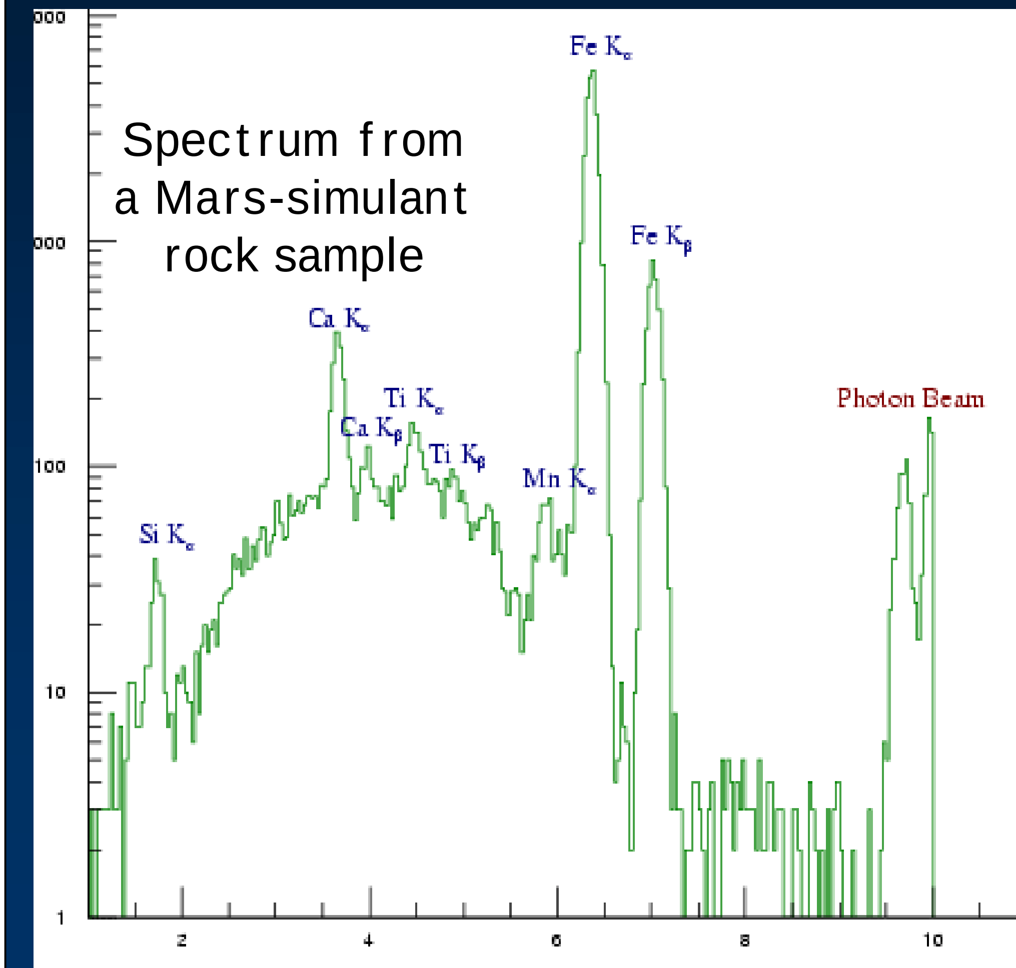


Fluorescence

Microscopic validation:
against reference data



Experimental validation:
test beam data, in collaboration with
ESA Advanced Concepts & Science
Payload Division



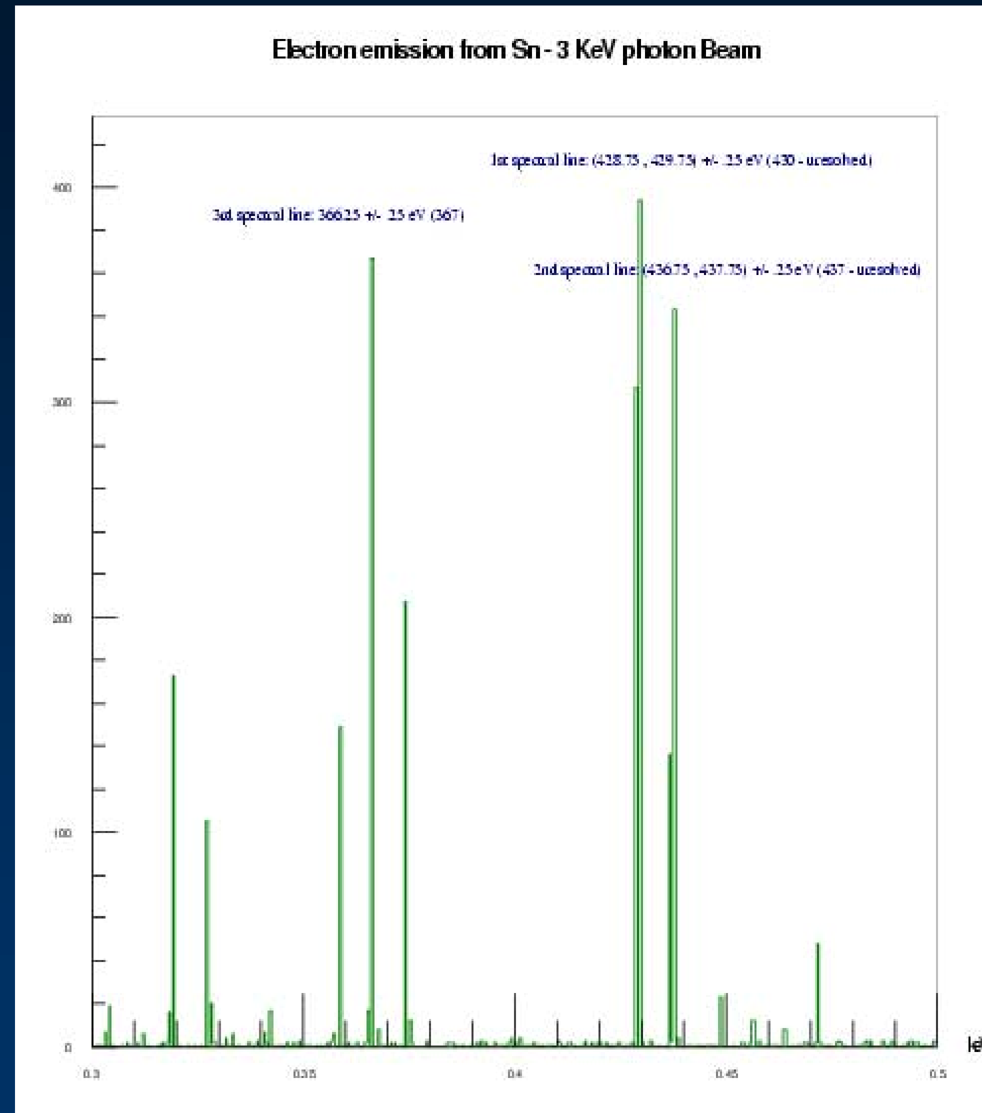
Auger effect

New implementation, validation in progress

Auger electron emission from various materials

Sn, 3 keV photon beam,

electron lines w.r.t. published experimental results



Recent development
Penelope processes

Processes à la Penelope

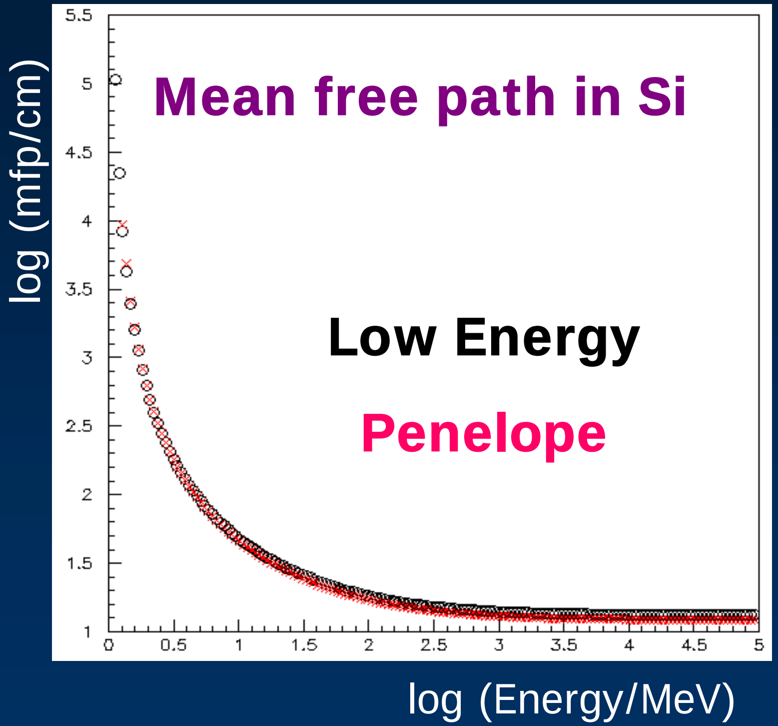
- Physics models by F. Salvat et al., implemented in a FORTRAN Monte Carlo code
  – the physics models have been **specifically developed** and a great care was dedicated to the **low energy description** (atomic effects, etc.): the (declared) lower limit is **100 eV**

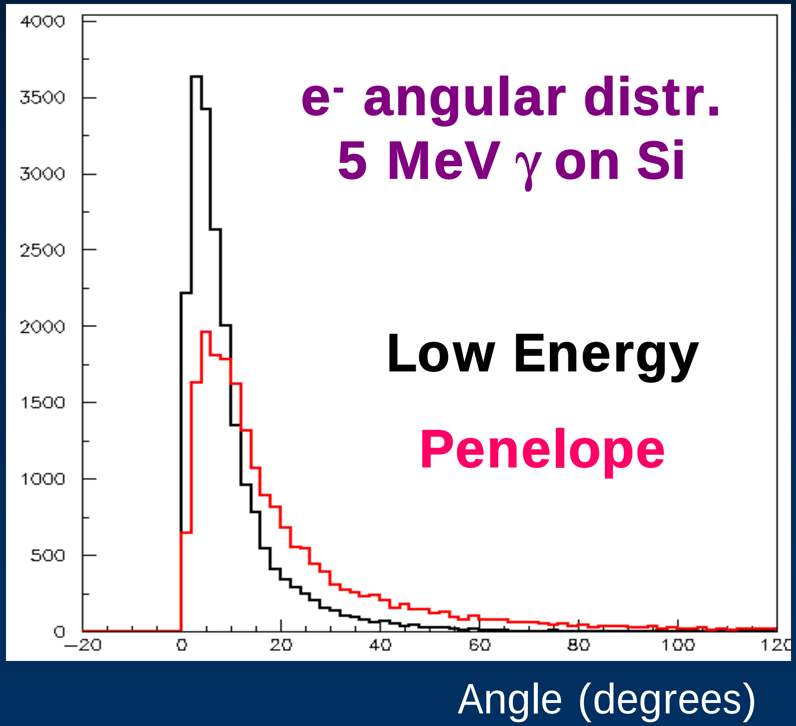
- The whole physics content of the Penelope Monte Carlo code has been re-engineered into Geant4 (except for multiple scattering)
  – processes for photons: release 5.2, for electrons: release 6.0

- Power of the OO technology:
  – extending the software system is easy
  – all processes obey to the same abstract interfaces
  – using new implementations in application code is simple

- Profit of Geant4 advanced geometry modeling, interactive facilities etc.
  – same physics as original Penelope

Gamma conversion

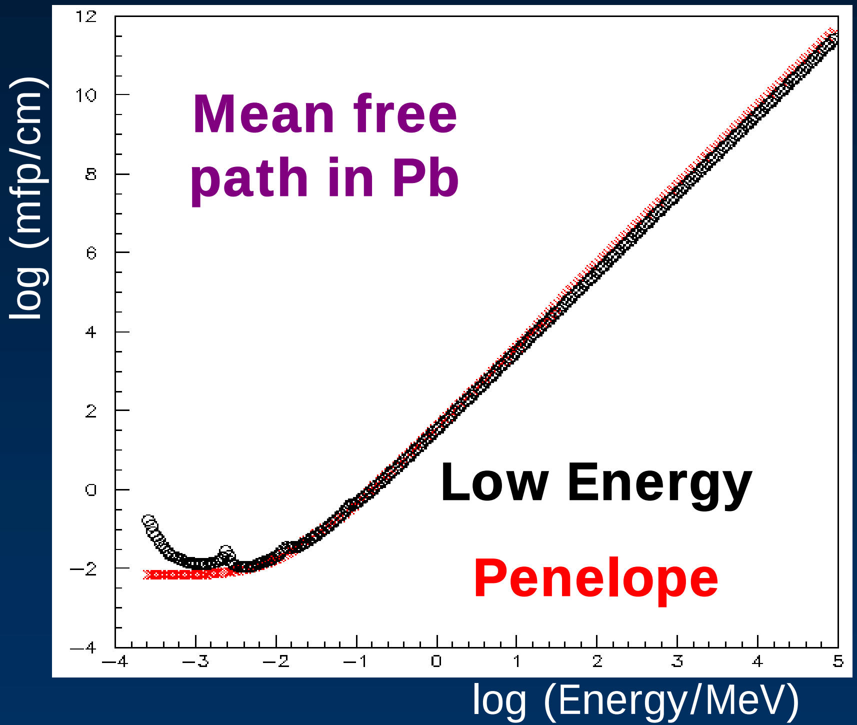


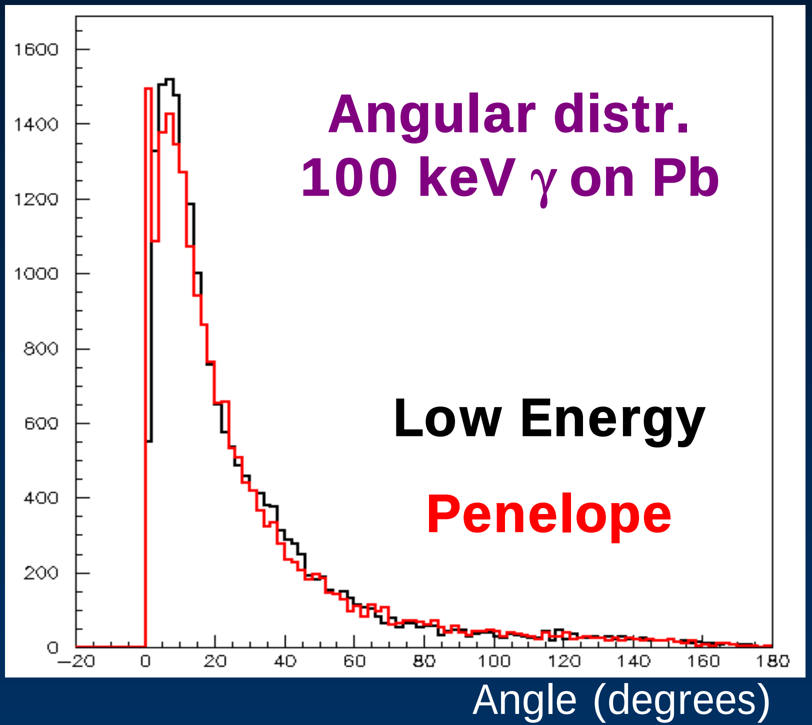


The cross sections are read from **database**

Analytical parametrisation of the final state

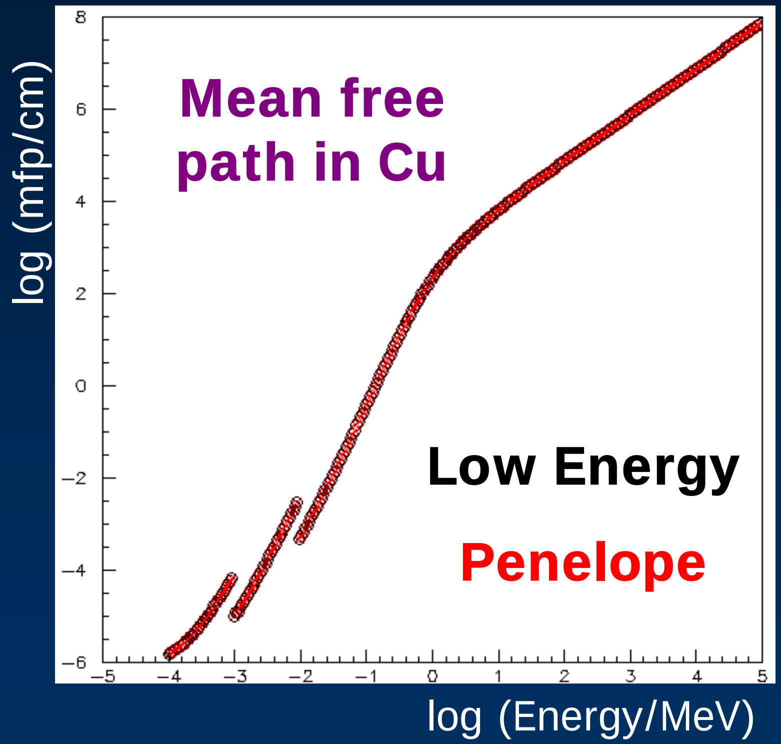
Rayleigh scattering

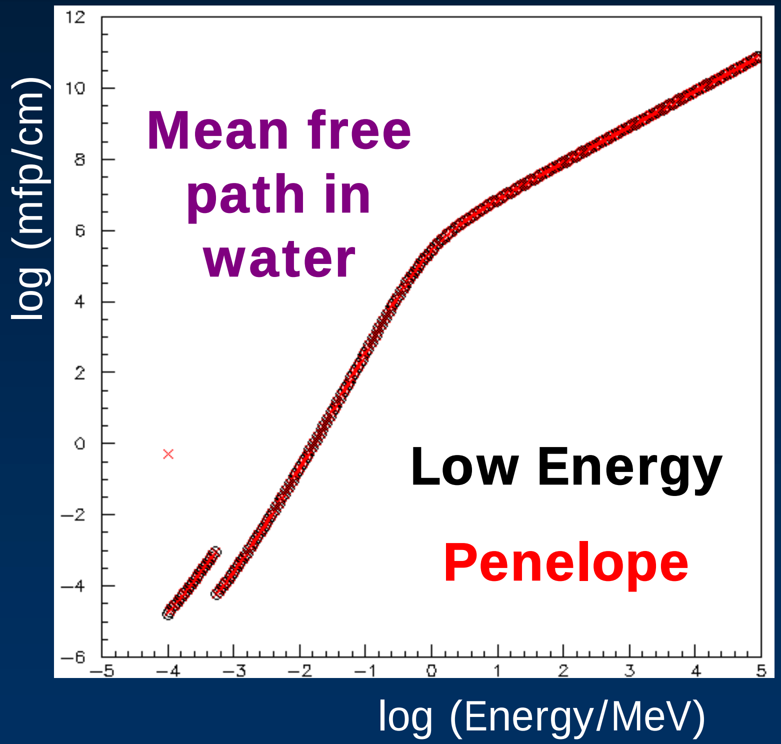




The cross sections are calculated using an **analytical parametrisation**: this requires numerical integrations and/or interpolations

Photoelectric effect

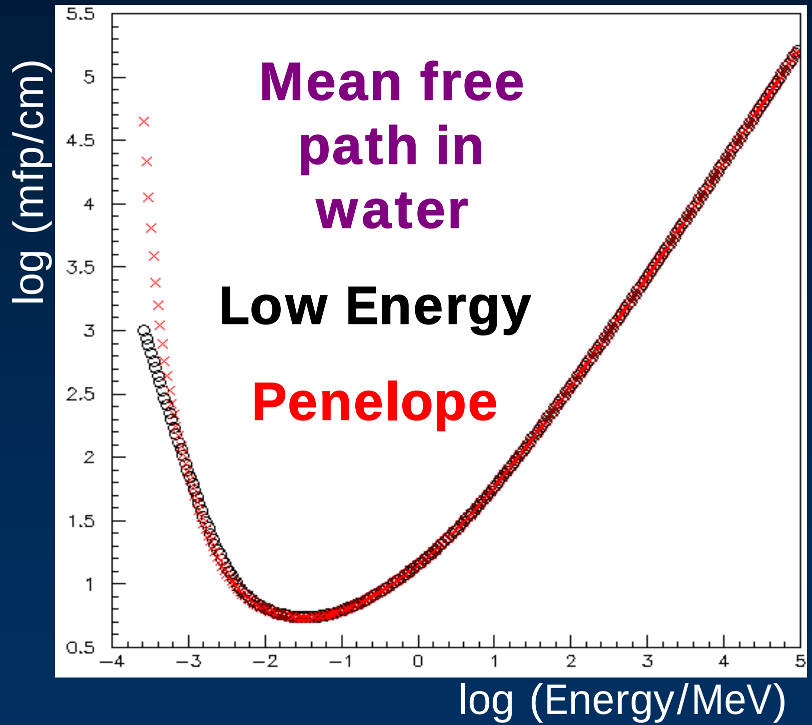


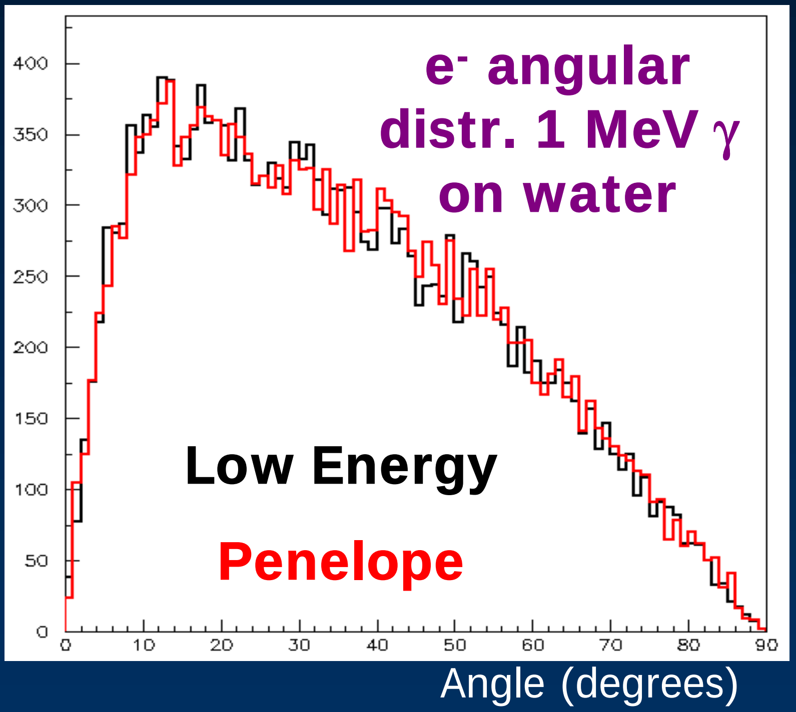


The cross sections are read from the **database**

Interfaced with G4 fluorescence classes (same secondaries)

Compton scattering



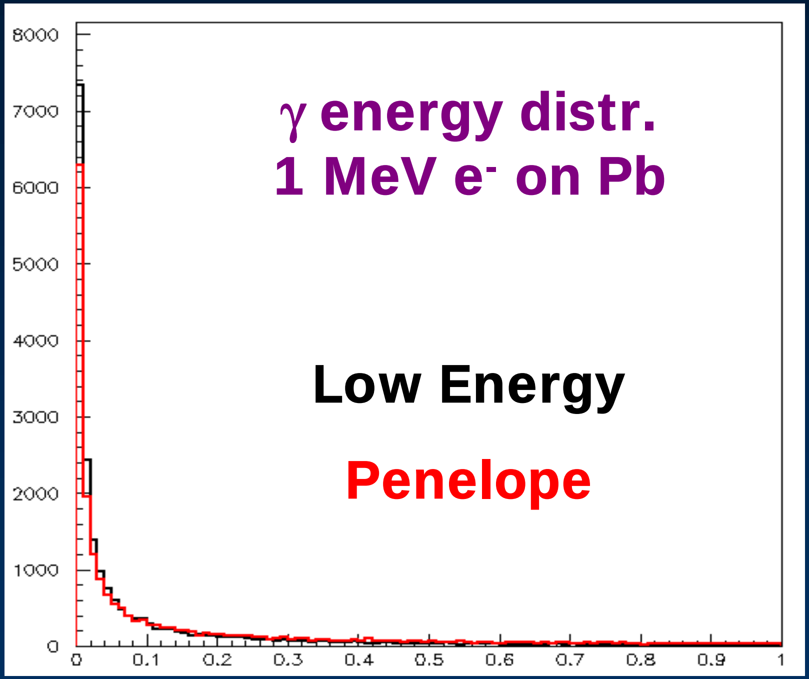


Analytical parametrisation for the cross section

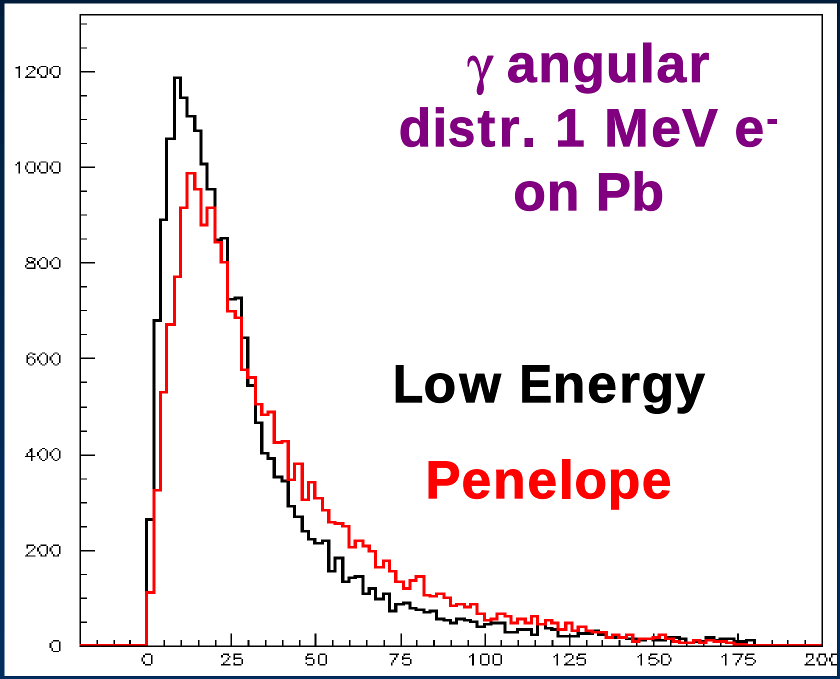
The model also predicts which atomic level is ionised

→ **fluorescence generation** (not present in LowE)

Bremssrahlung (electrons)



Relative γ energy



Angle (degrees)

γ **energy spectrum f(Z,E_{el}) → database** (as in G4LowEnergyBremsstrahlung, but 32 points instead of 15)

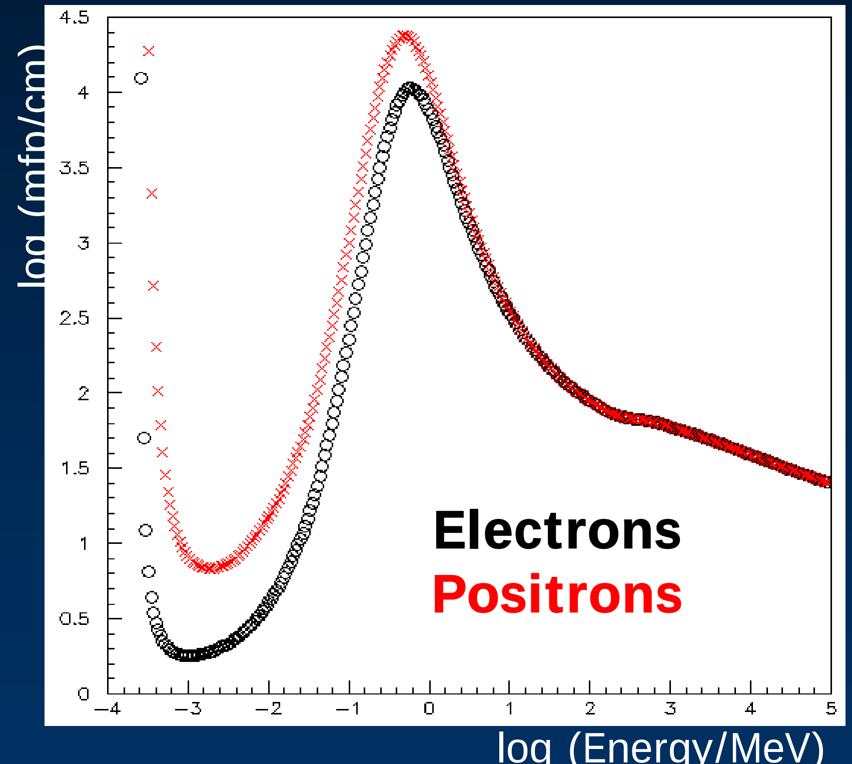
Also the **angular distribution** is **data-driven**

Bremsstrahlung (positrons)

It is assumed:

$$\frac{d\sigma^{(+)}}{dEdW} = g(Z,E)\frac{d\sigma^{(-)}}{dEdW}$$

g(Z,E) → parametrised correction function, independent of the γ energy W



The γ energy spectrum and the angular distribution are the **same as for electrons**, only the **cross section changes**

Validation

- Relative comparison LowE-Livermore/Penelope only for curiosity
  - helpful to understand effects of different modeling approaches
  - and to identify software bugs!
- Validation against experimental data
  - LowE-Livermore and Penelope processes both subject to the same validation process
  - more later...

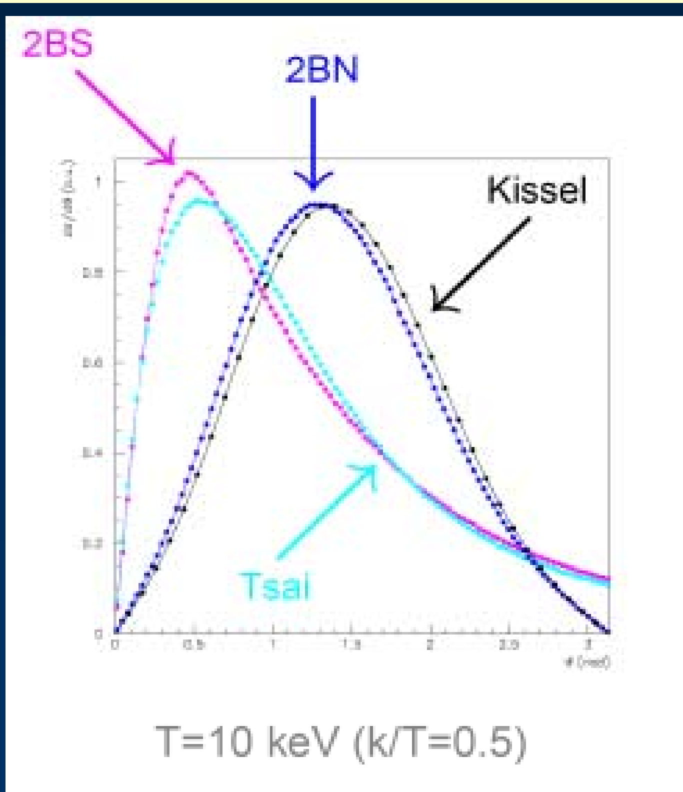
New development
Precise angular distributions

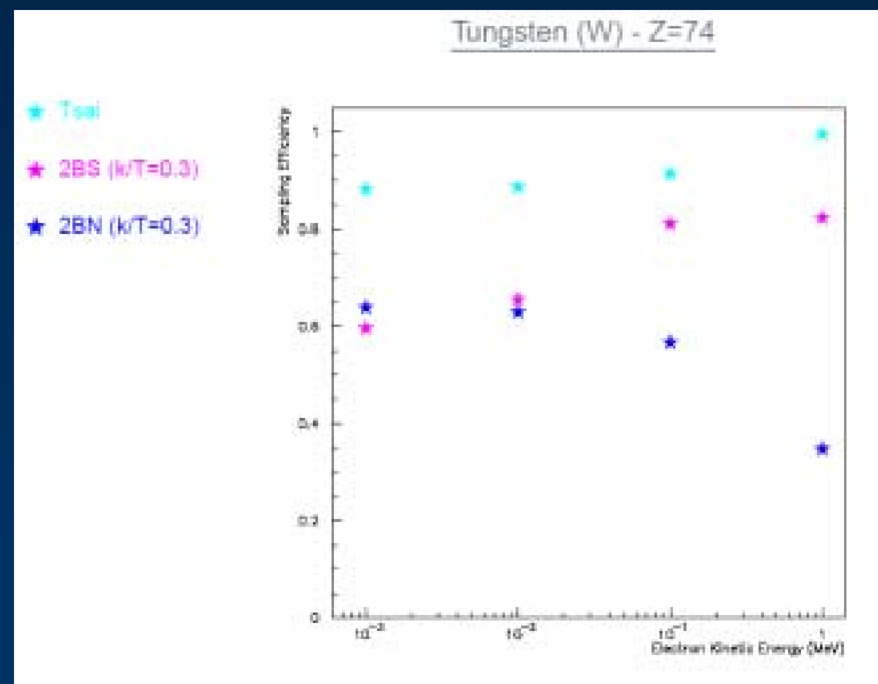
Bremsstrahlung Angular Distributions

Three LowE generators available in GEANT4 6.0 release:

G4ModifiedTsai, G4Generator2BS and G4Generator2BN

G4Generator2BN allows a correct treatment at low energies (< 500 keV)





Bremsstrahlung Angular Distributions

Open issues and news

- Large initialization time for G4Generator2BN *(see Physics Manual for details)*
  - use of pre-calculated data (reduces initialization time to zero)
  - introduced in Geant4 6.1

- Switching mechanism between different generators
  - design iteration for final state planned in July 2004
  - time scale for re-implementation and test compatible with Geant4 7.0, but priorities for 7.0 are currently still under discussion

Photoelectric Angular Distributions

Current status of photoelectric angular distributions in GEANT4.6.0

G4 LowE and LowE PENELOPE processes:

The incident photon is absorbed and one electron is emitted in the same direction as the primary photon

G4 Standard (*a la* GEANT3):

The polar angle of the photoelectron is sampled from an approximate Sauter-Gavrila cross-section (for K-shell)

PENELOPE:

The polar angle is sampled from K-shell cross-section derived from Sauter. The same cross-section is used for other photoionization events.

EGSnrc: Controlled by a master flag IPHTER

IPHTER = 0 (similar to G4 LowE)

IPHTER = 1 (Sauter distribution valid for K-shell)

Both assume that azimuthal angle distribution is uniform (no polarization)

Photoelectric Angular Distributions

to be released in 2004

Sauter formalism is valid for light-Z, K-shell photoelectrons and non-polarized photons

In progress: use a more generalized approach based on Gavrila theory

Valid for all-Z elements, for photoelectrons emitted from K and L shells also includes the effect of the polarization of the incident photon

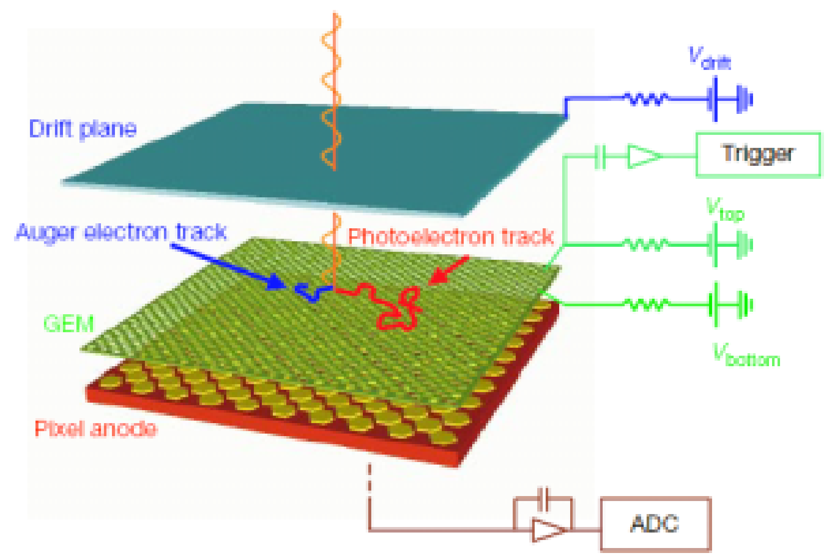
This enhancement is of significance importance for the design of experiments that aim to measure the polarization of X-rays emitted from black holes and neutron stars.

letters to nature

An efficient photoelectric X-ray polarimeter for the study of black holes and neutron stars

Enrico Costa*, Paolo Soffitta*, Ronaldo Bellazzini†, Alessandro Brez†, Nicholas Lumb† & Gloria Spandre†

* *Istituto di Astrofisica Spaziale del CNR, Via Fosso del Cavaliere 100, I-00133, Rome, Italy*
† *Istituto Nazionale di Fisica Nucleare-Sezione di Pisa, Via Livornese 1291, I-56010 San Piero a Grado, Pisa, Italy*



NATURE | VOL 411 | 7 JUNE 2001 | www.nature.com

New development
PIXE

PIXE in Geant4

- A preliminary model for fluorescence emission induced by hadrons has been implemented in Geant4 for ~1 year
  - based on a theoretical model for the calculation of cross sections
    - M. Gryzinski, Two-Particle Collision. I. General Relations for Collisions in the Laboratory System, Phys. Rev. vol. 138, no. 2A, 19 April 1965
    - M. Gryzinski, Two-Particle Collision. II. Coulomb Collisions in the Laboratory System of Coordinates, Phys. Rev. vol. 138, no. 2A, 19 April 1965
- Subject to systematic test only recently
  - a software bug has been discovered in the implementation of the model
  - ...but, more important: **the theoretical model is not adequate**

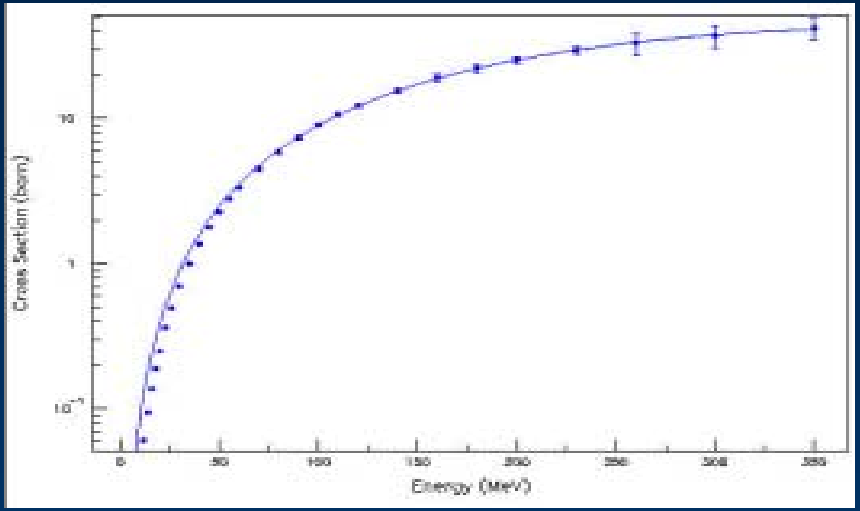
New PIXE model

- New approach: parameterised model based on compilations of data
- Compilation of cross sections for protons and ions by H. Paul (Univ. Linz)
  - H. Paul and J. Sacher, Fitted Empirical Reference Cross Sections for K-Shell Ionization by Proton, Atomic and Nucl. Data Tables 42, 105-156, 1989
- The range of energy is between 5 KeV and 500 MeV
- The range of elements covered is from C to U

PIXE Development: the new model

- Data are fit; fit results, rather than original data, are used to predict the value of a cross section at a given hadron/ion energy
  - allows extrapolations to lower/higher E than data compilation
  - *same approach may be explored also for faster X-ray fluo model*

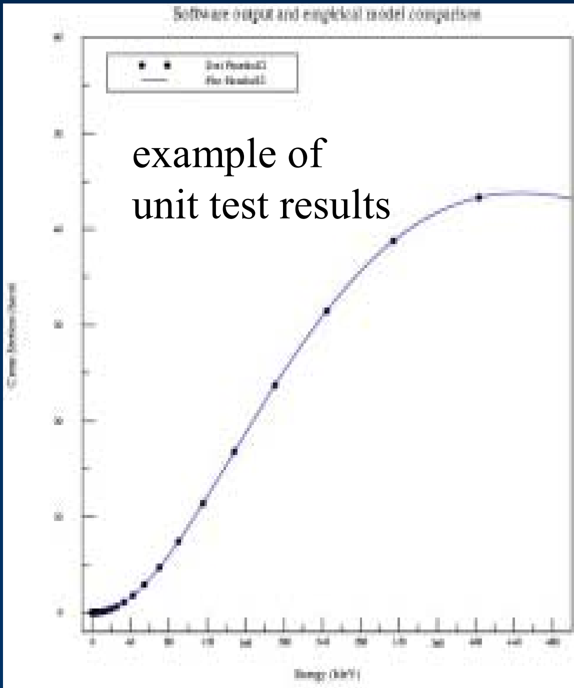
- The best fit is with three parametric functions for three different groups of elements depending on the atomic numbers:
  - $6 \leq Z \leq 25$
  - $26 \leq Z \leq 65$
  - $66 \leq Z \leq 9$



  - the only exception of this scheme is Cl (Z=17); reference data for Cl are best fit by the function for the second group of elements ($26 \leq Z \leq 65$)

Status and future developments

- First implementation for protons, K-shell
  - to be released with Geant4 6.2, 25 June 2004
  - preliminary model *(1 function fits)* already implemented, unit tested, currently under integration test
  - improved model *(2-3 function fits)* currently under unit test; to be released in summer reference tags (Geant4-beta)
- Second iteration: protons, L-shell
  - release planned for Geant4 7.0
- Third iteration: ions, K-shell
  - compilations of cross-sections limited to K-shell
  - release foreseen in early 2005



Other new developments

Ongoing...

- Regular maintenance and improvements in many areas
  - improved, precise calculation of range for hadrons and ions
  - extension of parameterised models for hadrons up to ~8 Mev
  - code review of Penelope processes
  - performance optimisation
  - improved treatment for some materials (i.e. graphite)
  - etc.

- Major design iteration on the whole LowE package
- Design iteration of atomic relaxation
  - spanned over 2004
  - closely associated to the "Test & Analysis" project (needs sound regression and physics testing)

Current major activity
Validation

Physics Tests

Electromagnetic physics
Standard, LowE, Penelope

- Particle CSDA range
- Particle Stopping Power
- Transmission coefficient
- Backscattering coefficient
- Photon Attenuation coefficient
- Cross sections
- Particle range
- Bremsstrahlung energy spectrum
- Multiple scattering distributions
- Energy deposit in absorber
- Bragg peak (including hadronic interactions)
- etc.

...and more

Test results

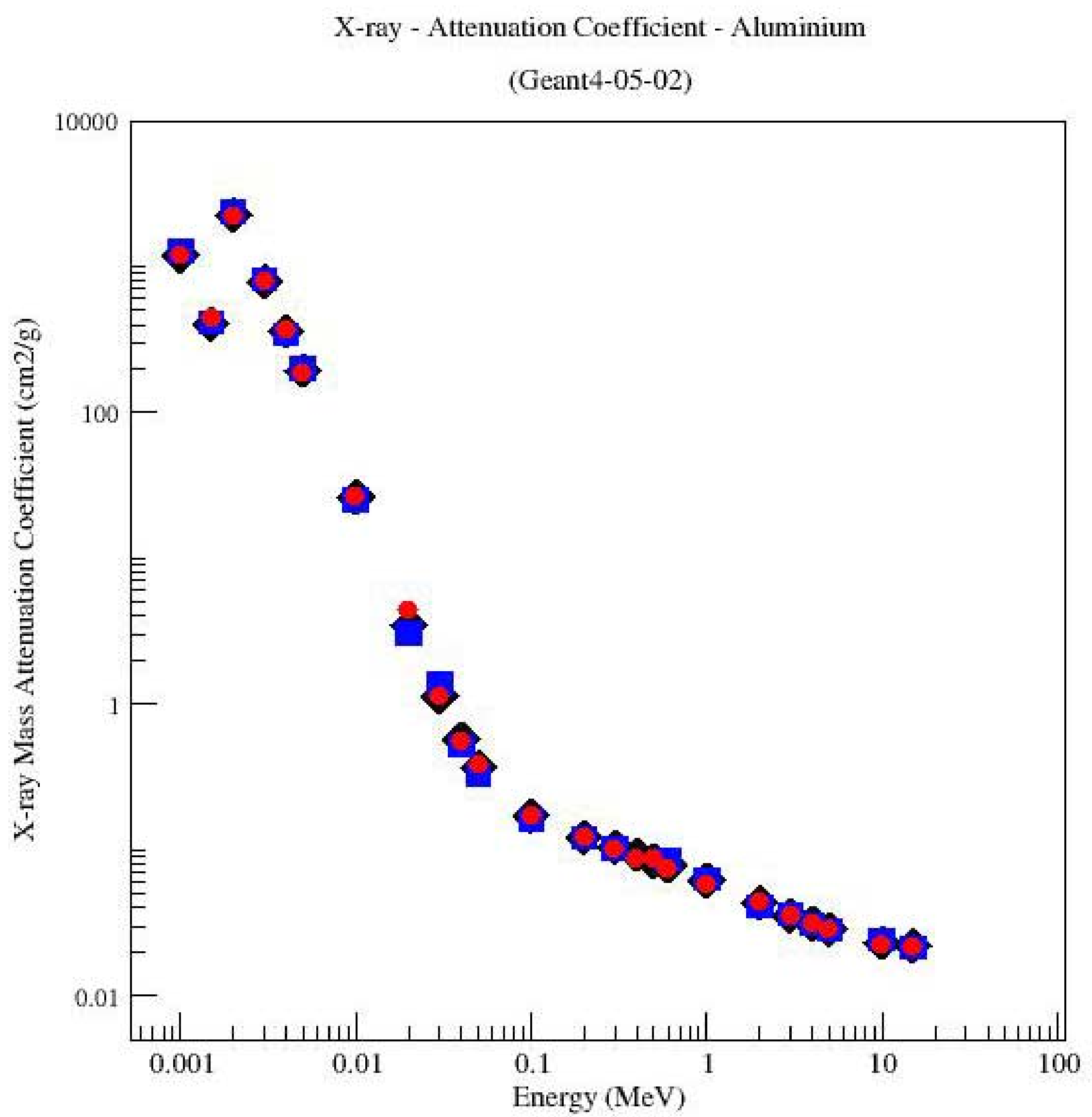
Photon attenuation coefficient

-ln (gammaTransmittedFraction / (targetThickness * absorberDensity))

Absorber Materials:

Be, Al, Si, Ge, Fe, Cs, Au, Pb, U

X-ray Attenuation Coefficient - Al



$\chi^2_{N\text{-}L}=13.1 - \nu=20 - p=0.87$

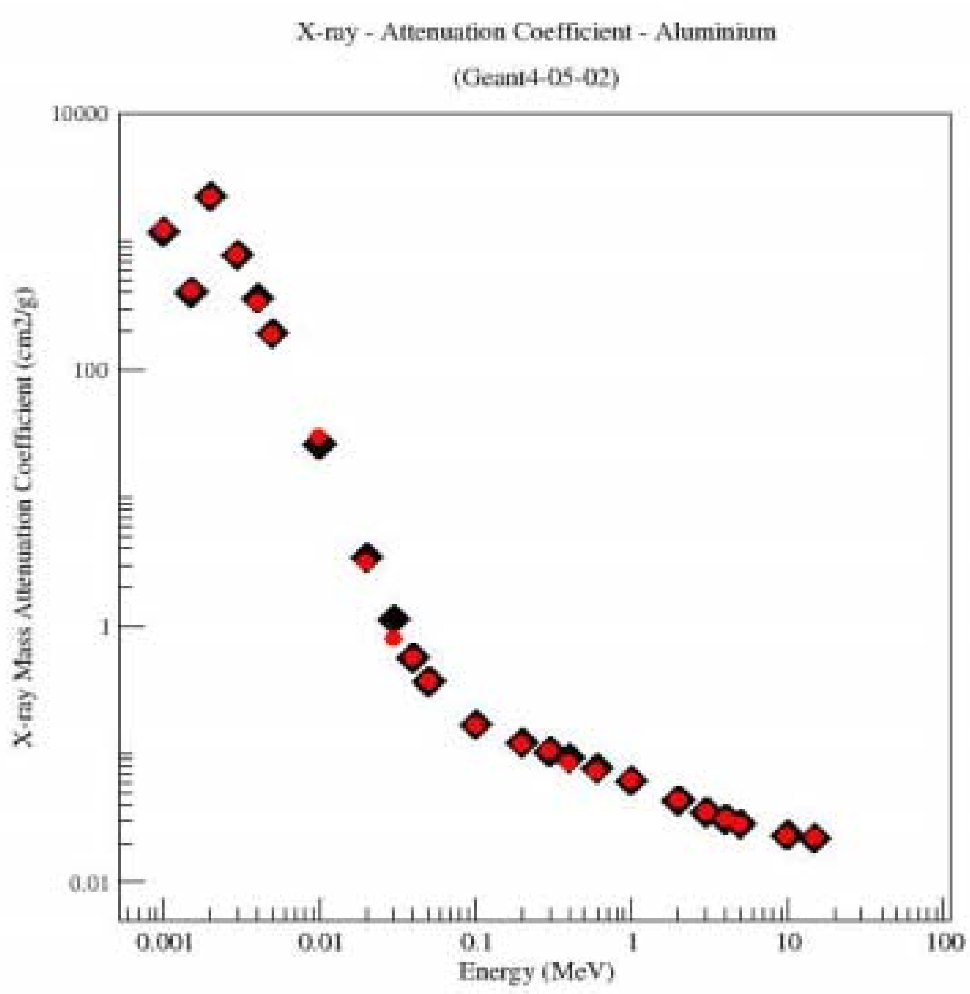
$\chi^2_{N\text{-}S}=23.2 - \nu=15 - p=0.08$

NIST-XCOM

G4 Standard

G4 LowE

X-ray Attenuation Coefficient - Al

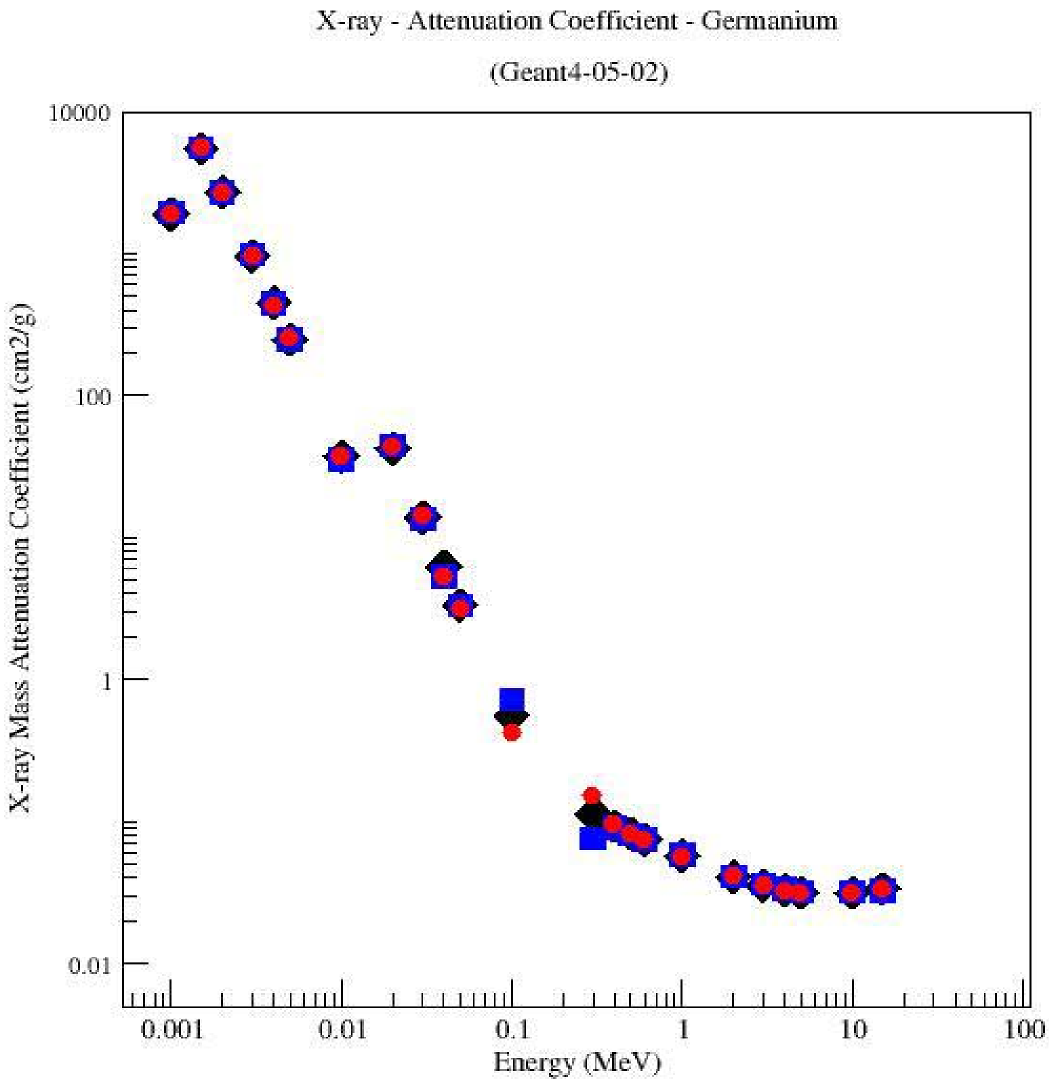


$\chi^2_{N-P}=15.9 - \nu=19 \quad p=0.66$

◆ NIST-XCOM

● G4 LowE Penelope

X-ray Attenuation Coefficient - Ge



$\chi^2_{N-L}=26.3 - \nu=23 - p=0.29$

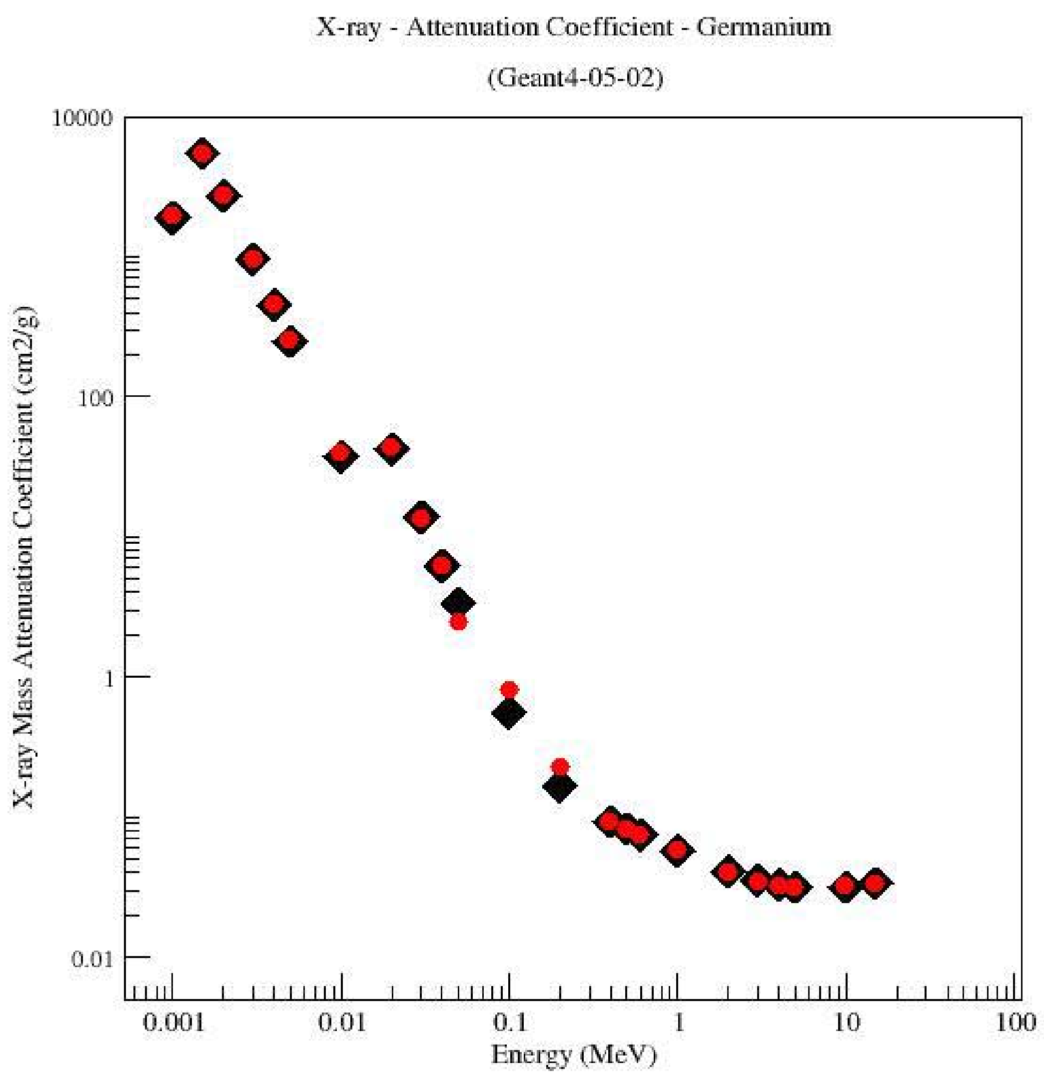
$\chi^2_{N-S}=27.9 - \nu=23 - p=0.22$

NIST-XCOM

G4 Standard

G4 LowE

X-ray Attenuation Coefficient - Ge

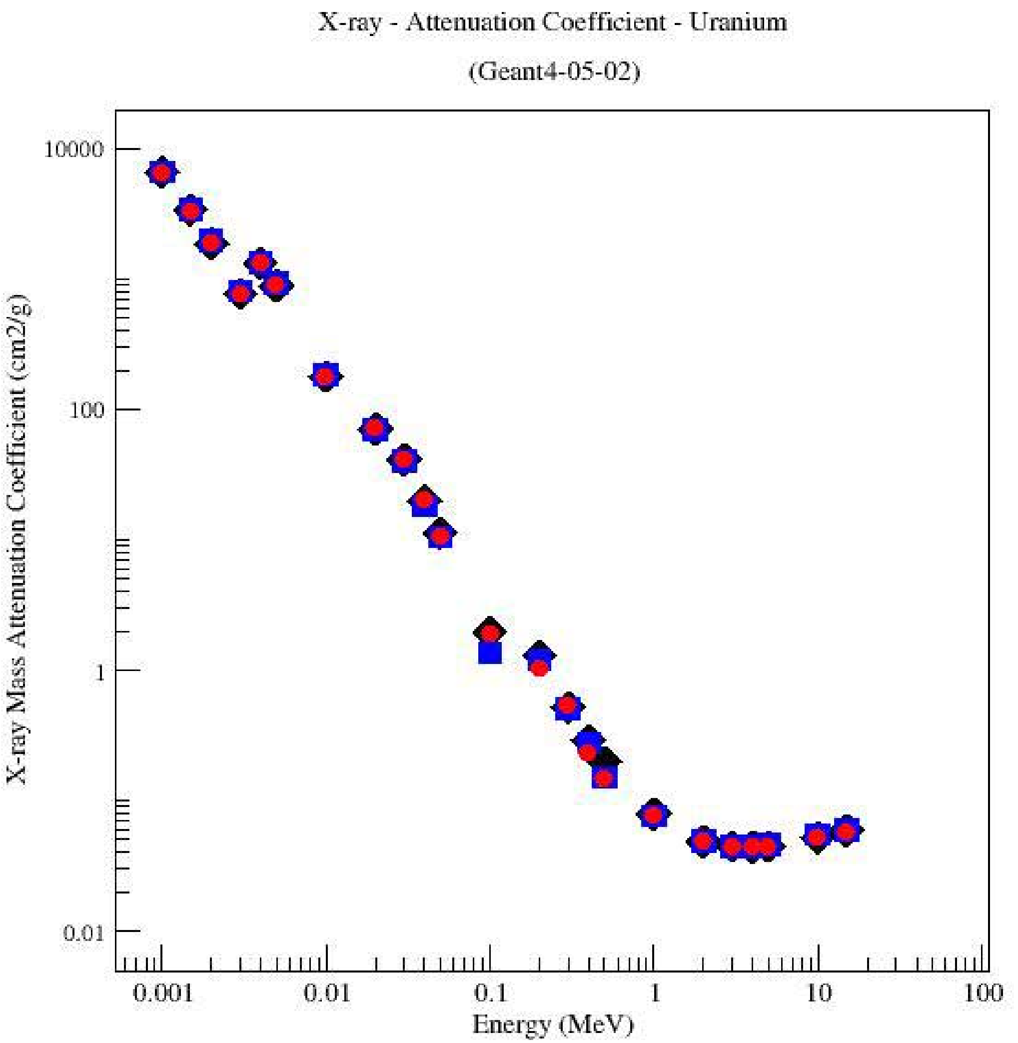


$\chi^2_{N-P}=10.1 - \nu=21 - p=0.98$

NIST-XCOM

G4 LowE Penelope

X-ray Attenuation Coefficient - U



$\chi^2_{N\text{-}L}=6.6 - \nu=20$ - $p=0.99$

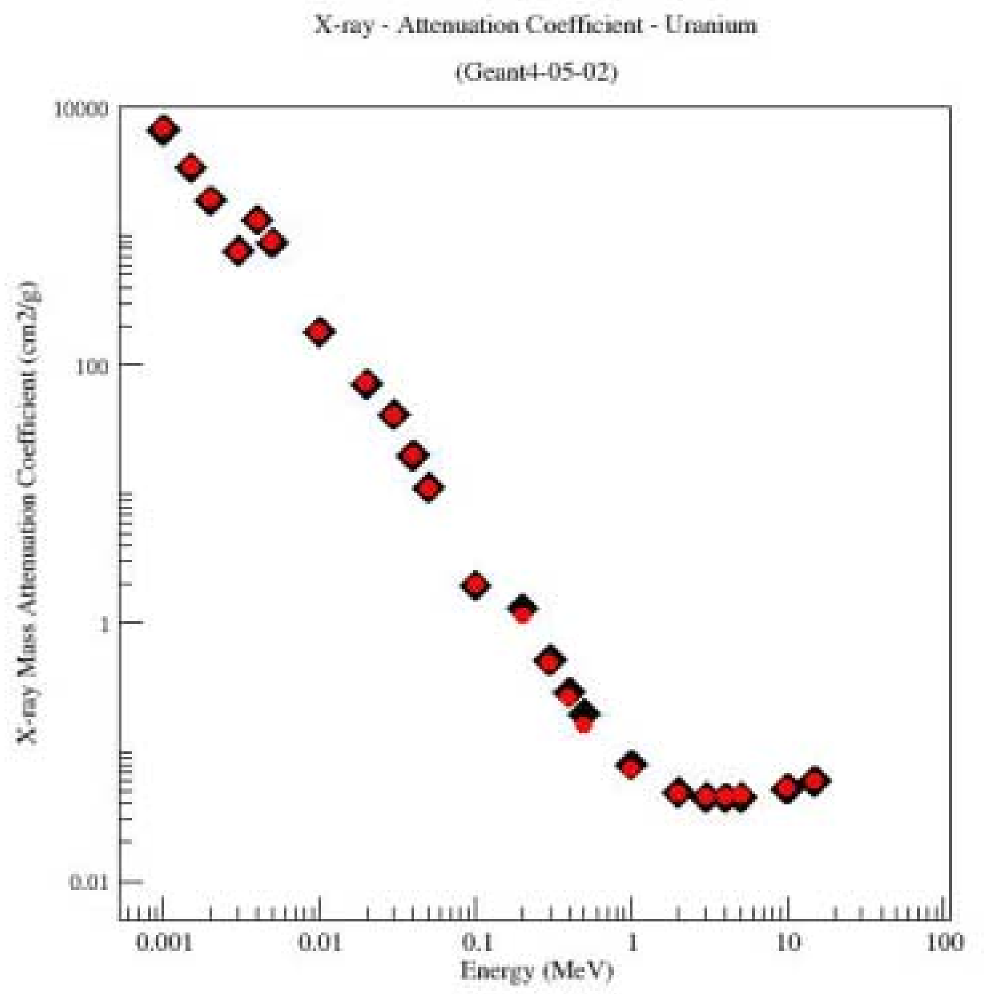
$\chi^2_{N\text{-}S}=14.7 - \nu=20$ - $p=0.80$

NIST-XCOM

G4 Standard

G4 LowE

X-ray Attenuation Coefficient - U



$\chi^2_{N-P}=19.3$ – $\nu=22$ - $p=0.63$

NIST-XCOM

G4 LowE Penelope

Test results

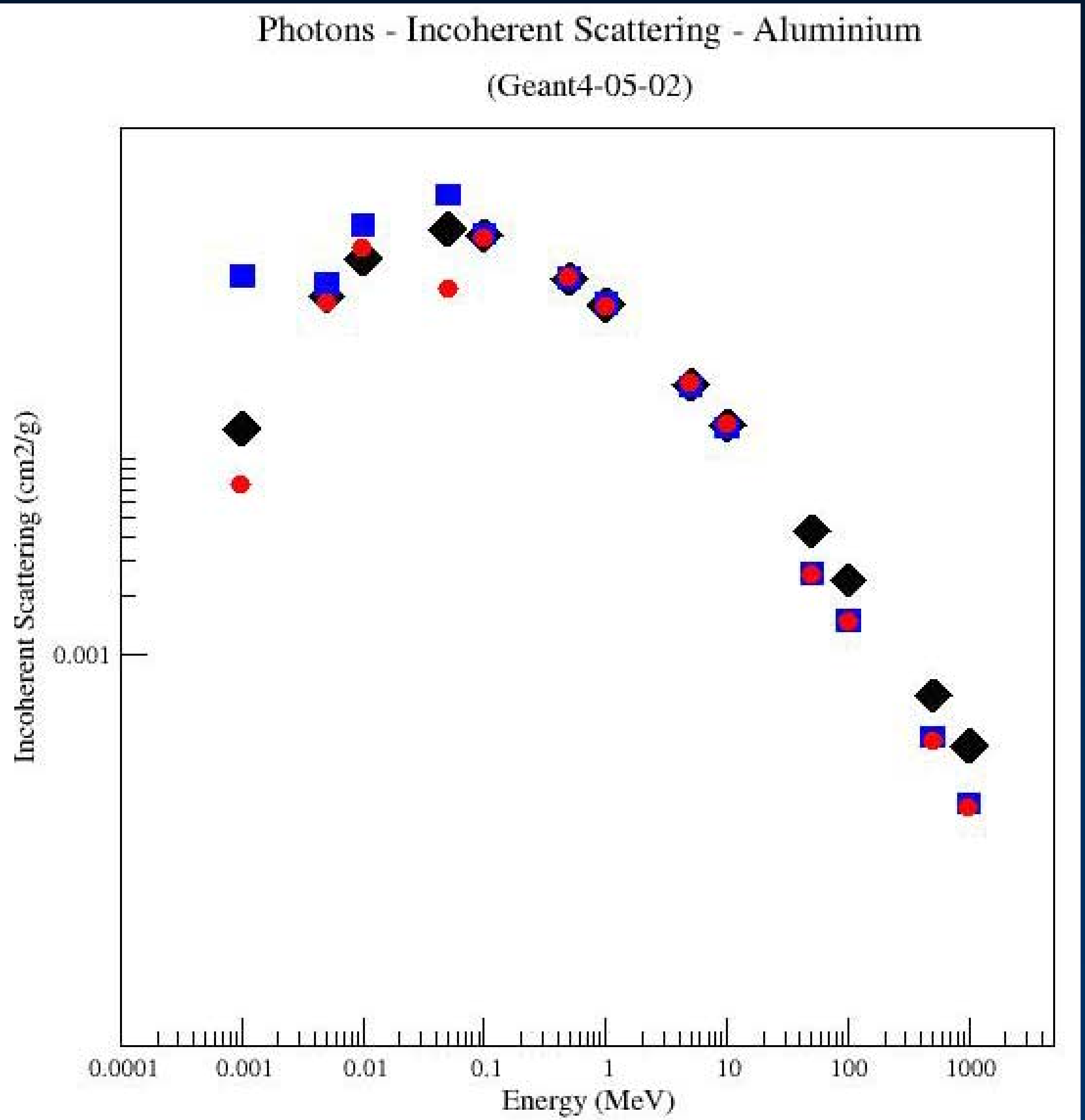
Photon cross sections

attenuation coefficients with only one process activated

Absorber Materials:

Be, Al, Si, Ge, Fe, Cs, Au, Pb, U

Compton Scattering - Al



$\chi^2_{N\text{-}L}$= 12.9– ν=8 - p=0.12

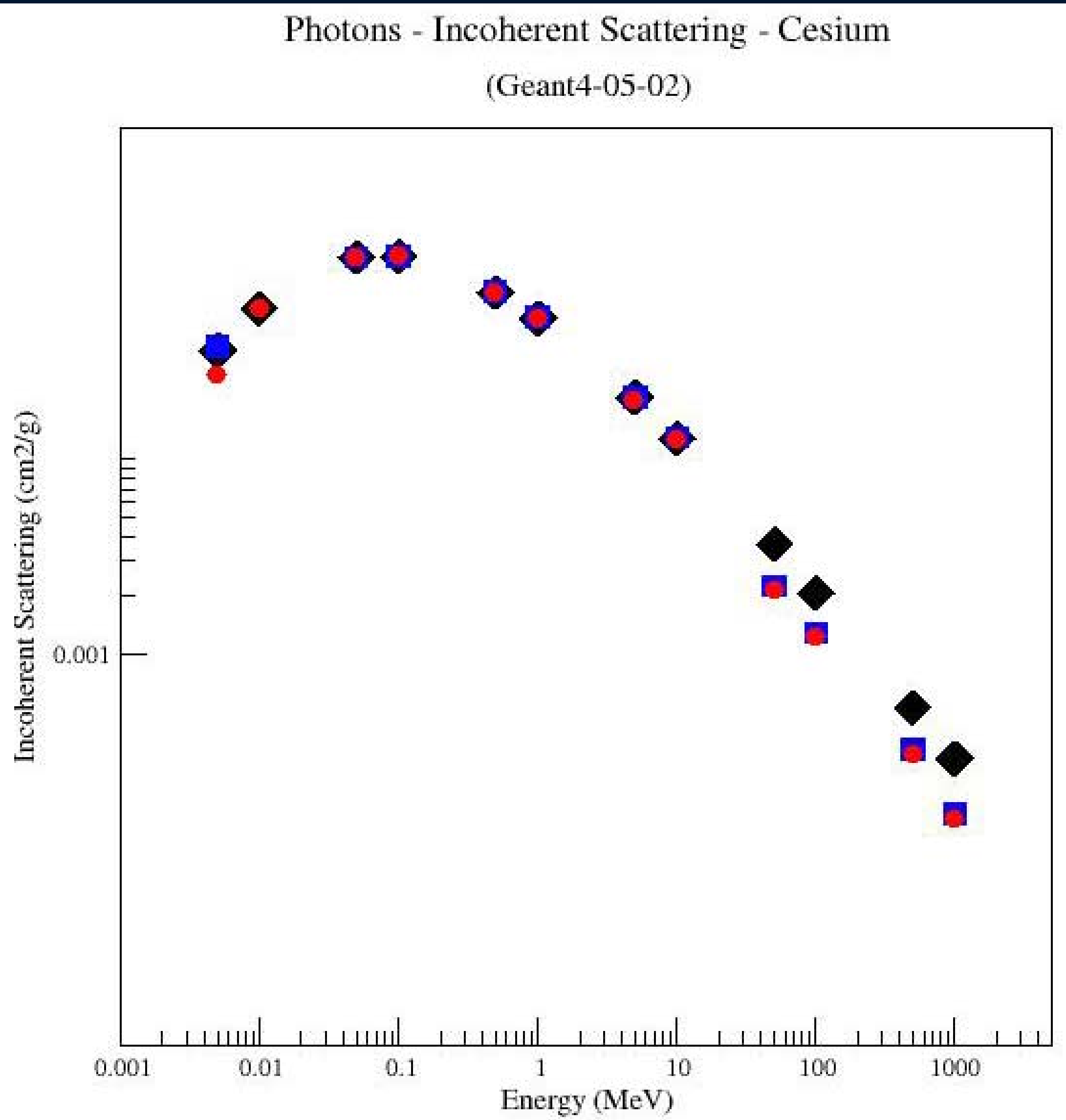
$\chi^2_{N\text{-}S}$=8.7 – ν=6 - p=0.19

NIST-XCOM

G4 Standard

G4 LowE

Compton Scattering - Cs



$\chi^2_{N\text{-}L}=4.6 - \nu=8$ - $p=0.80$

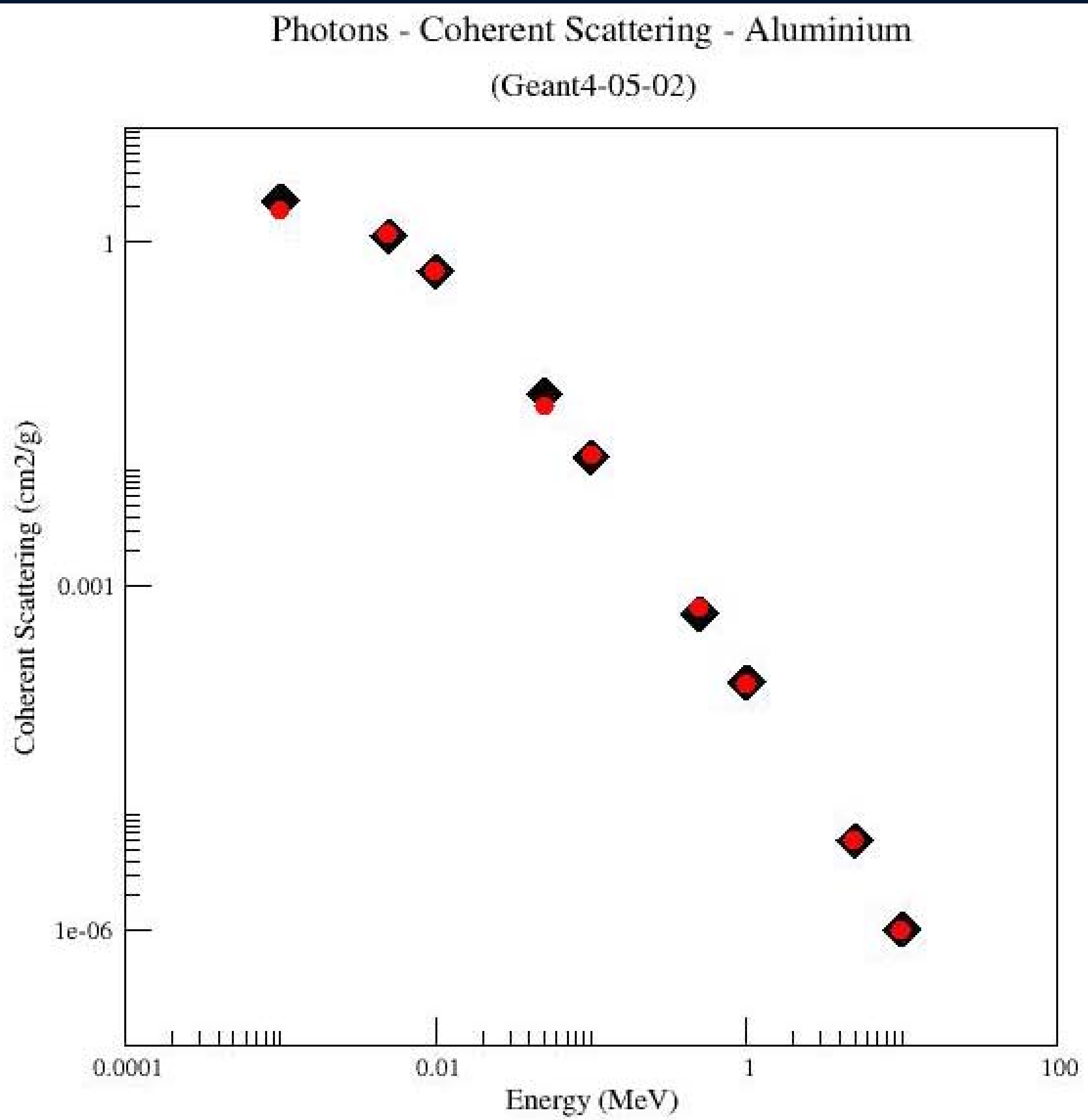
$\chi^2_{N\text{-}S}=1.8 - \nu=8$ - $p=0.99$

NIST-XCOM

G4 Standard

G4 LowE

Rayleigh Scattering - Al

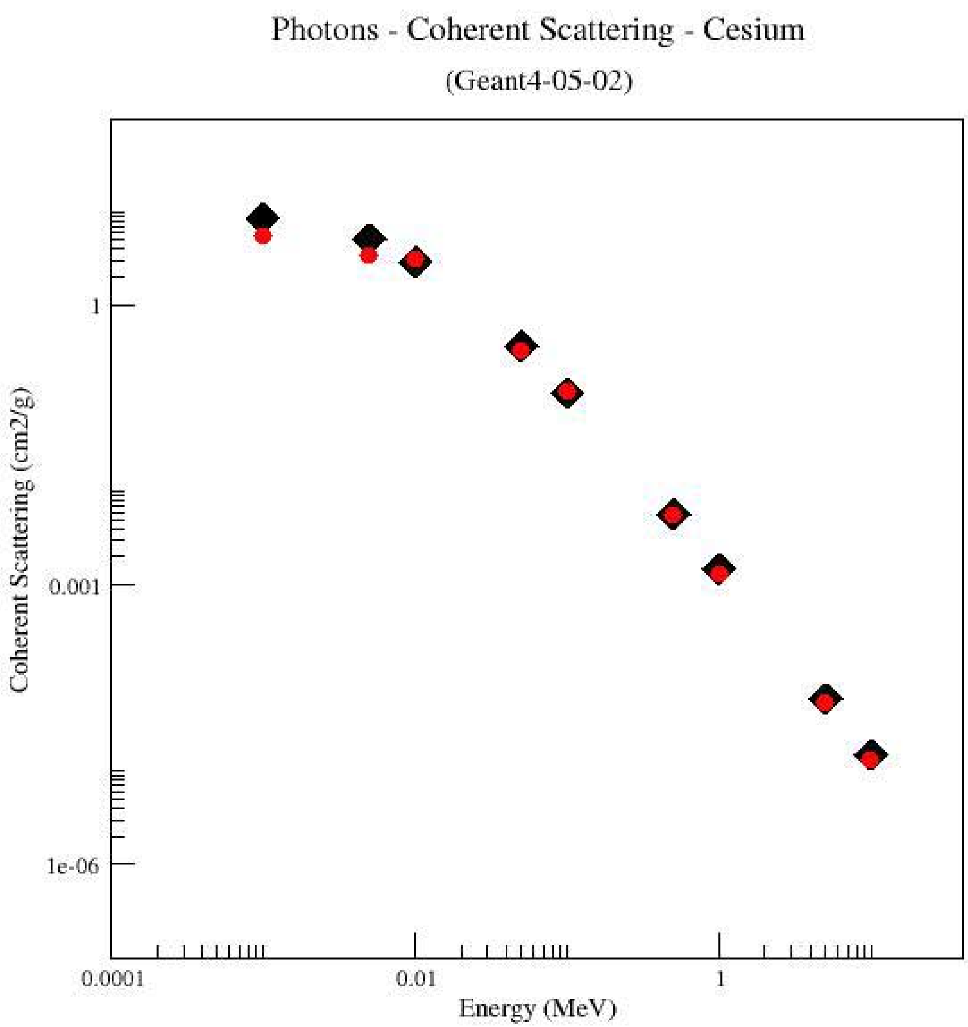


χ^2_{N-L}=13.6 – ν=11 - p=0.26

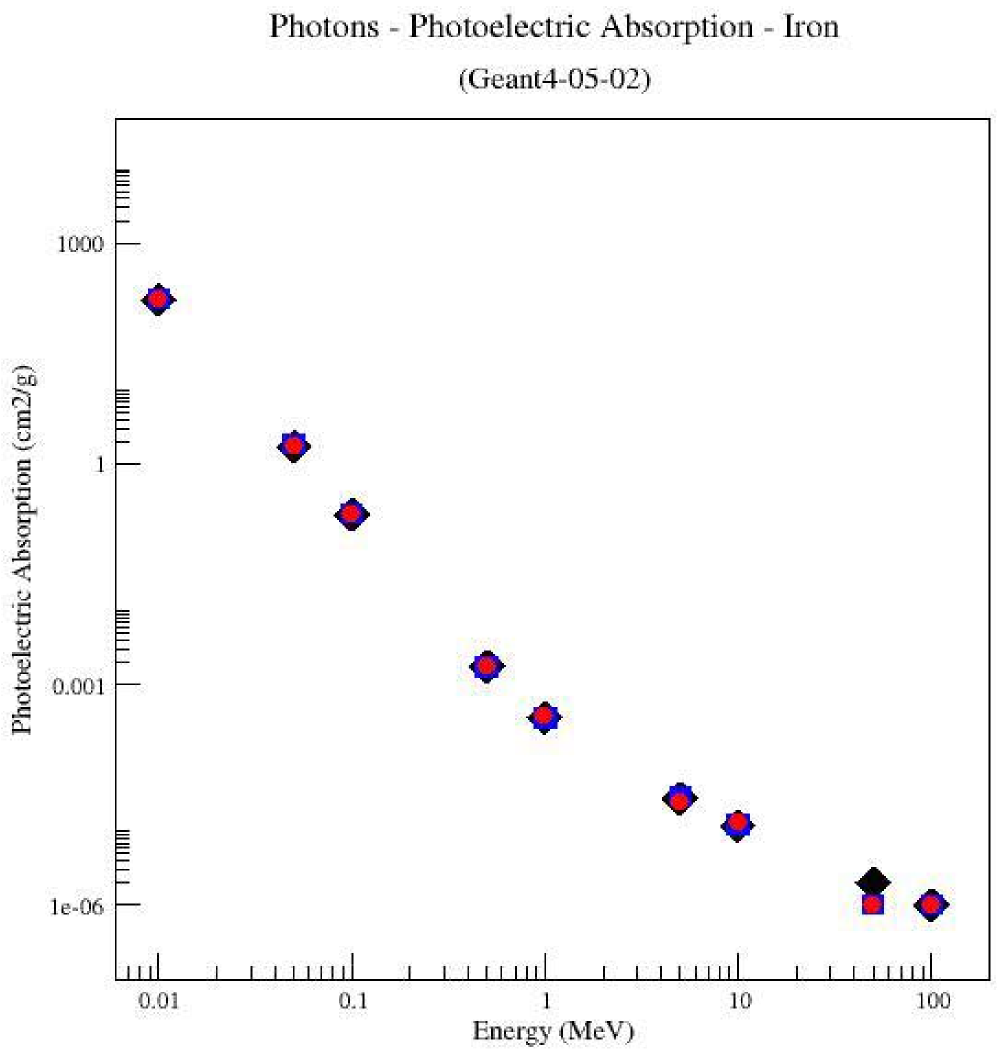
◆ NIST-XCOM

● G4 LowE

Rayleigh Scattering - Cs



Photoelectric Effect - Fe

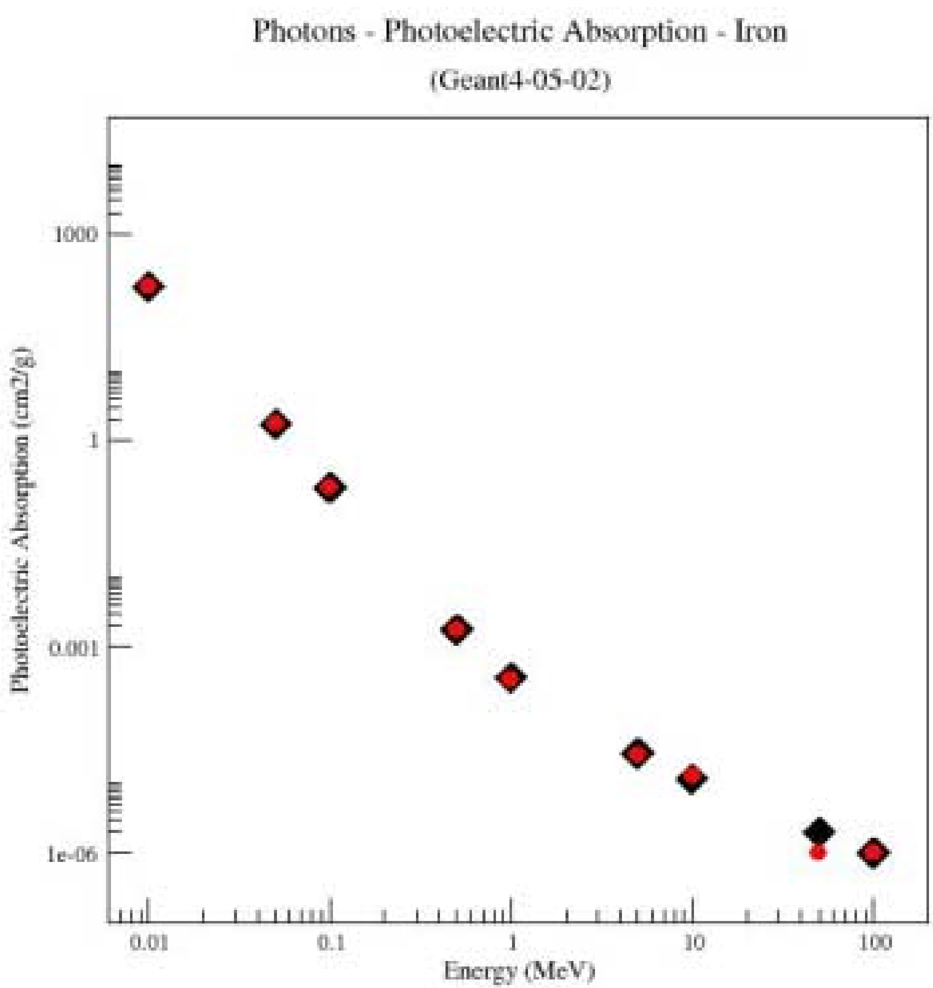


NIST-XCOM

G4 Standard

G4 LowE

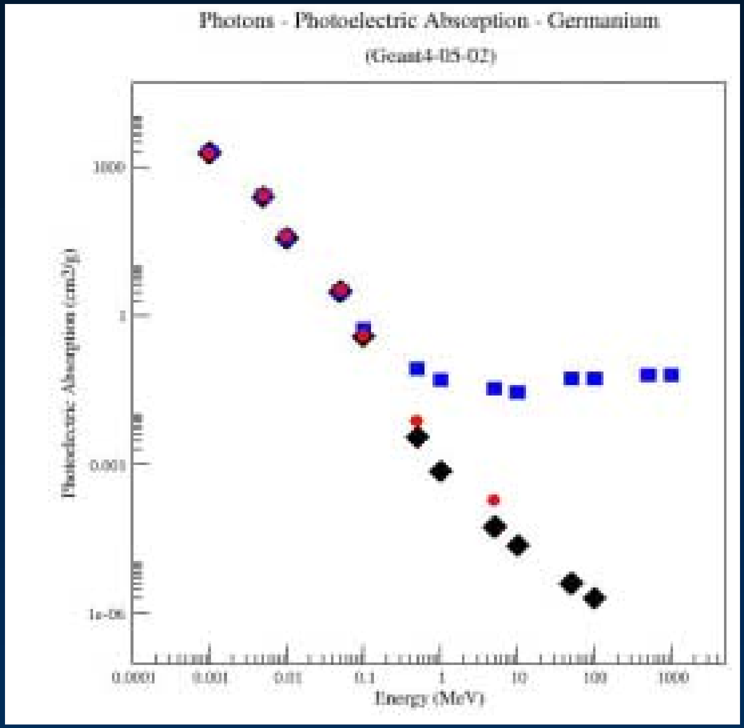
Photoelectric effect - Fe



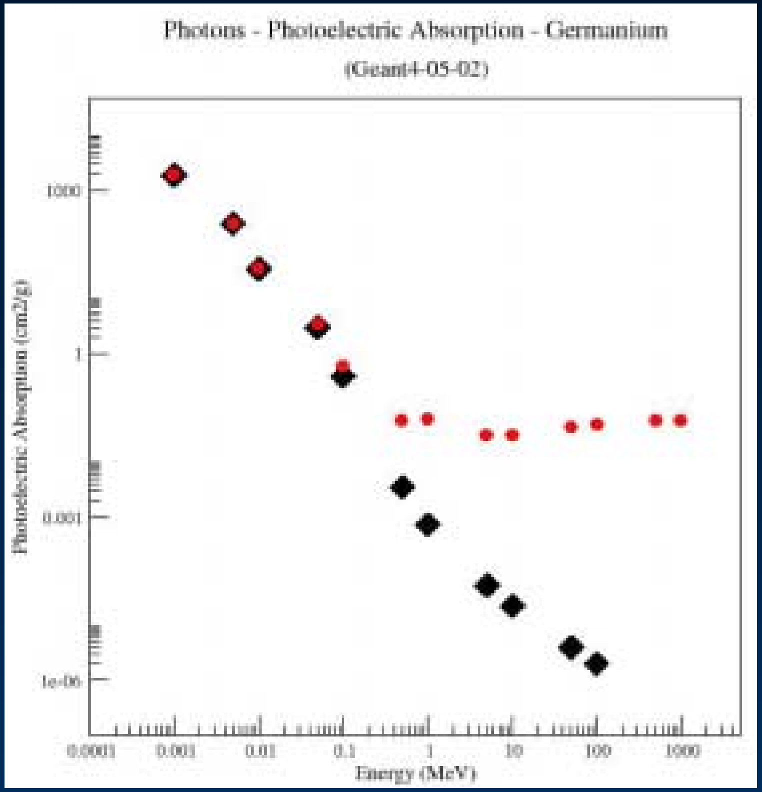
NIST-XCOM

G4 LowE Penelope

Photoelectric Absorption - Ge



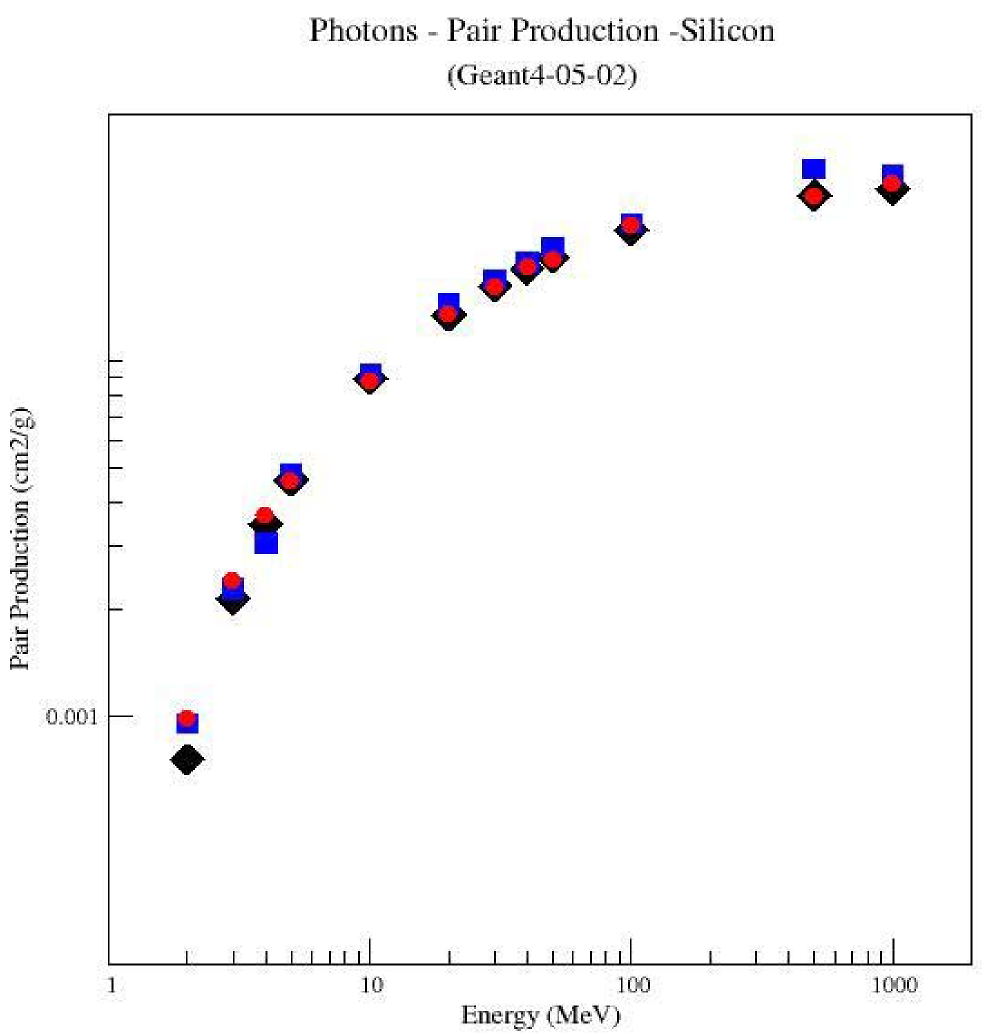
- NIST-XCOM
- G4 Standard
- G4 LowE



- NIST-XCOM
- G4 LowE Penelope

2 compatible Monte Carlo are not necessarily the Truth!

Pair Production - Si



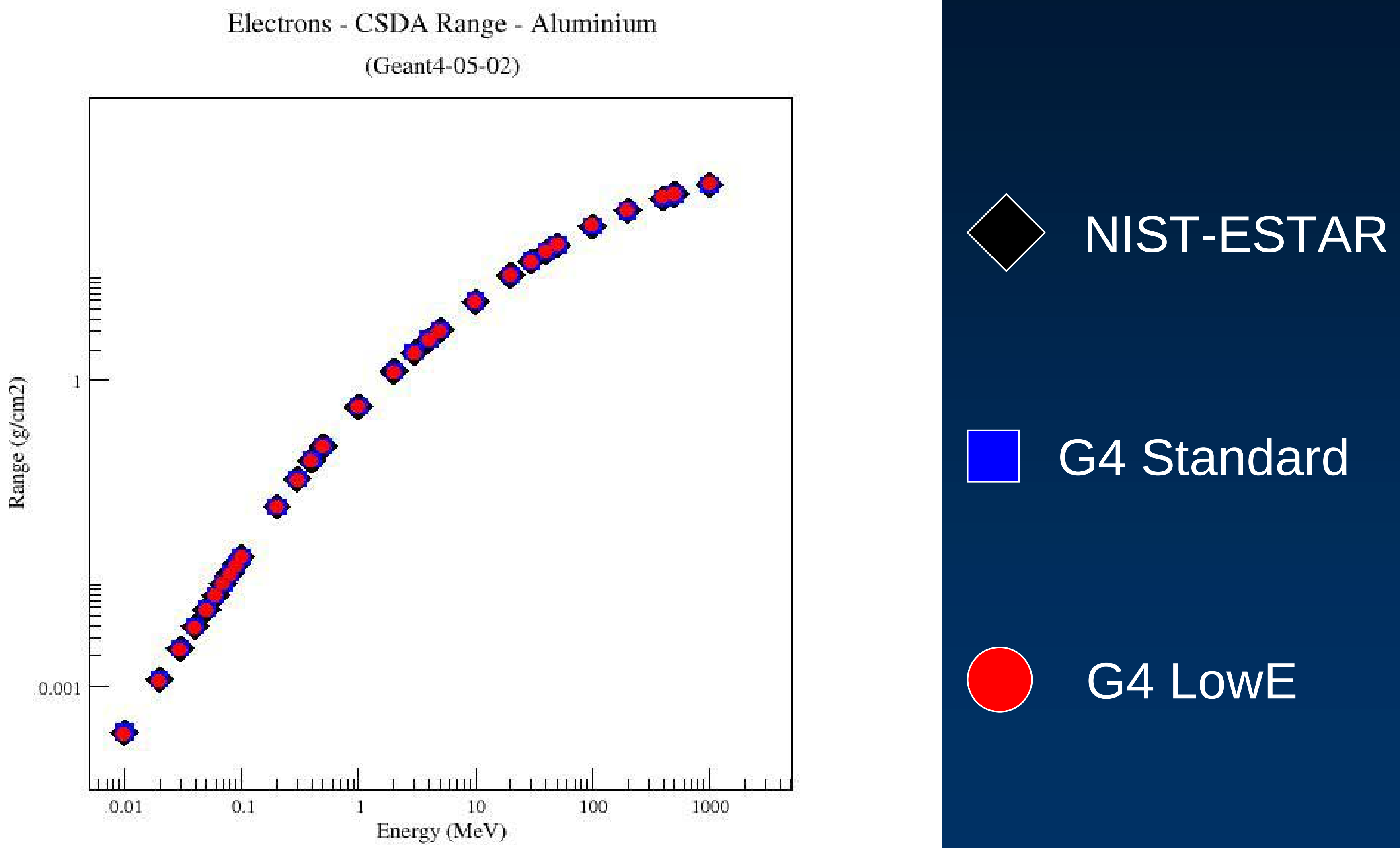
Test results

CSDA range and Stopping Power for electrons
- no multiple scattering
- no energy fluctuations

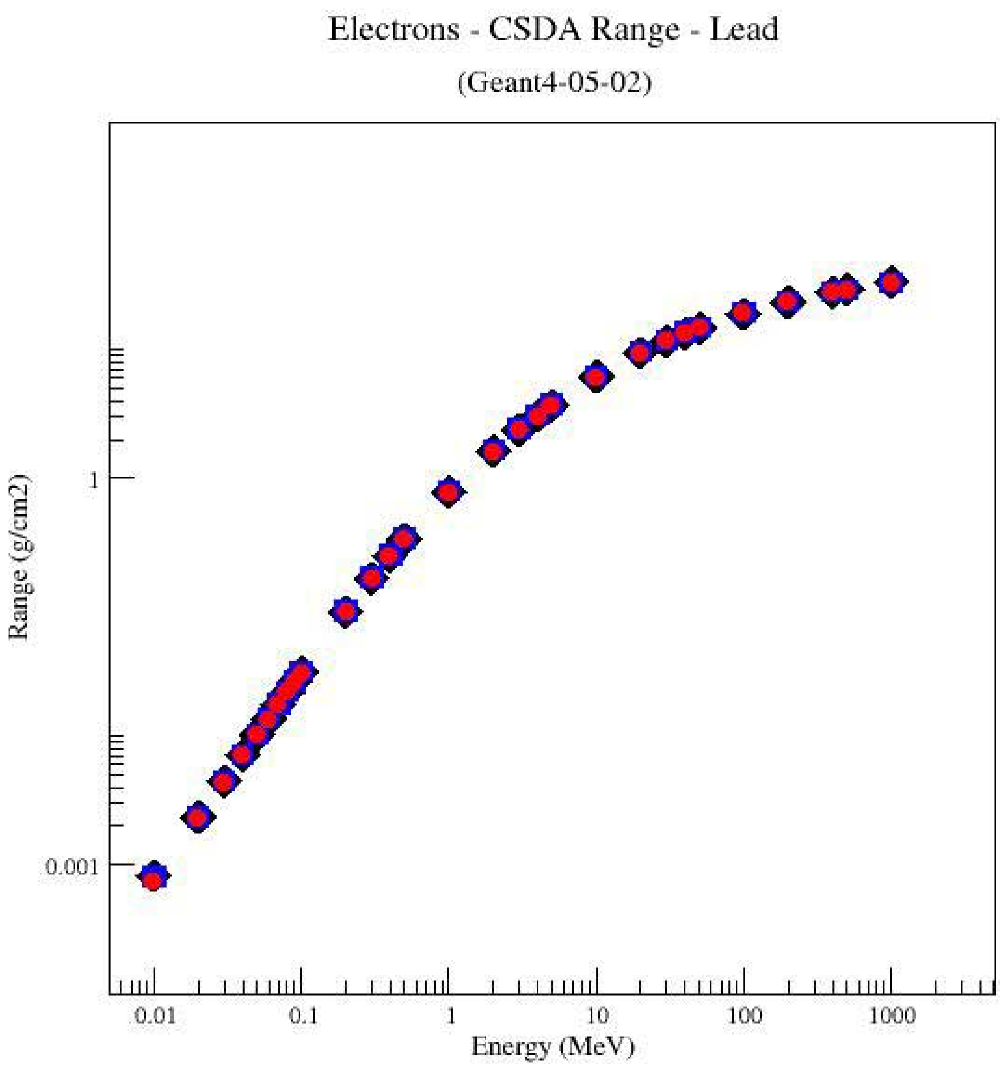
Absorber Materials:

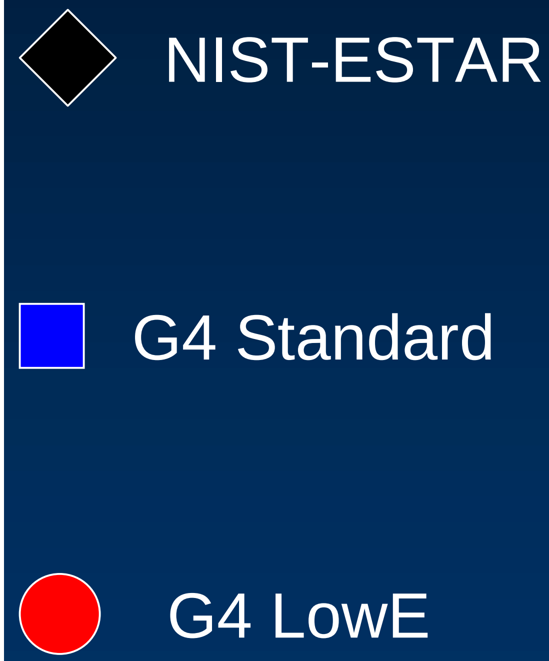
Be, Al, Si, Ge, Fe, Cs, Au, Pb, U

CSDA Range - Al

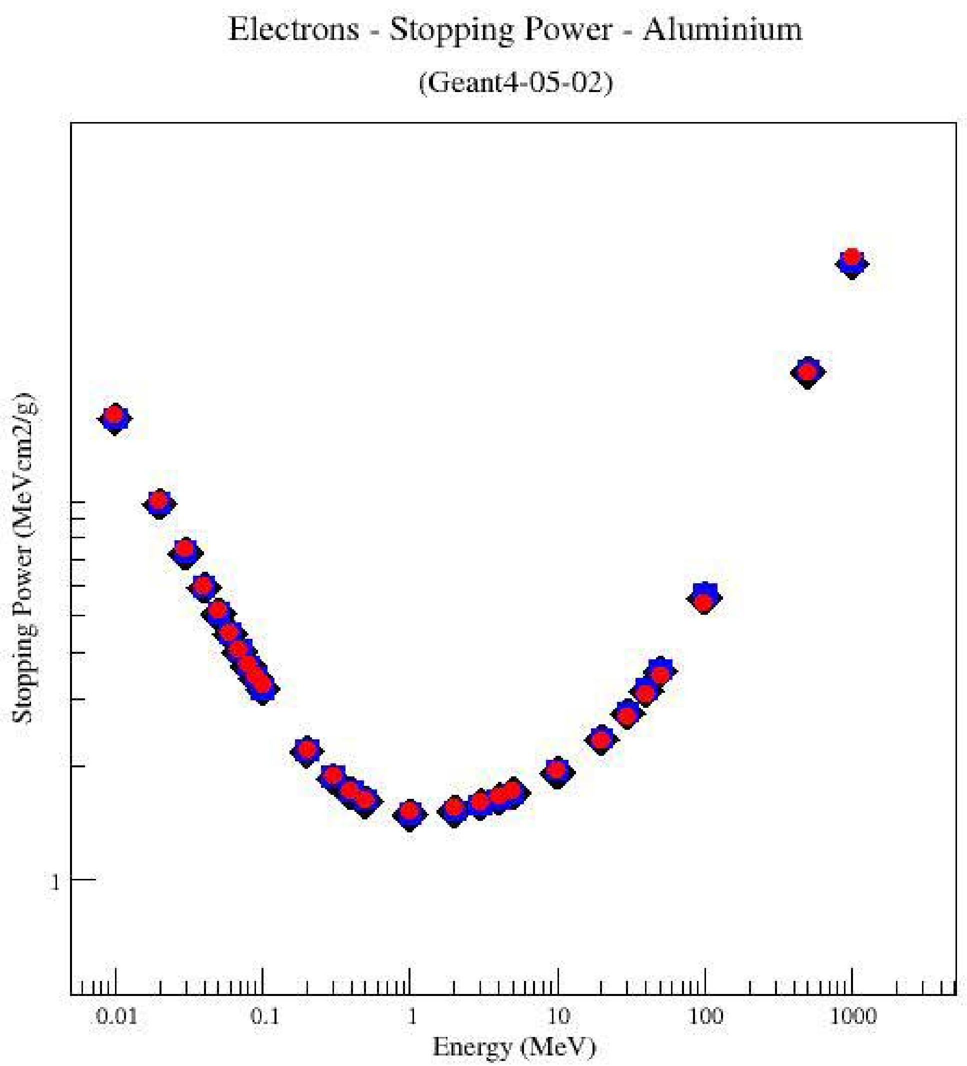


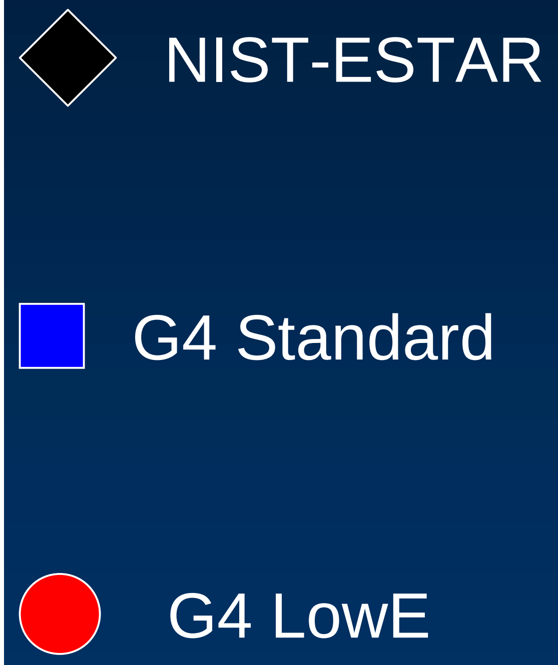
CSDA Range - Pb



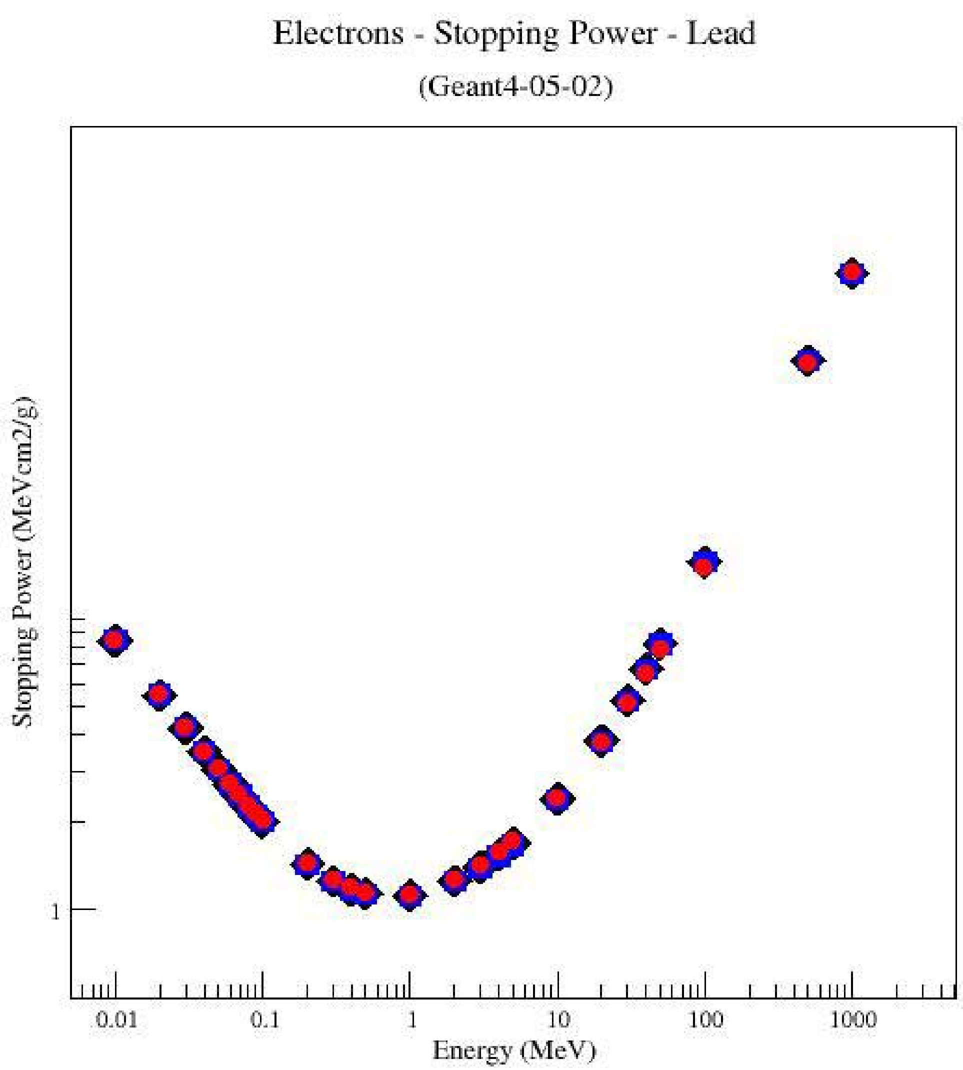


Stopping Power - Al





Stopping Power - Pb

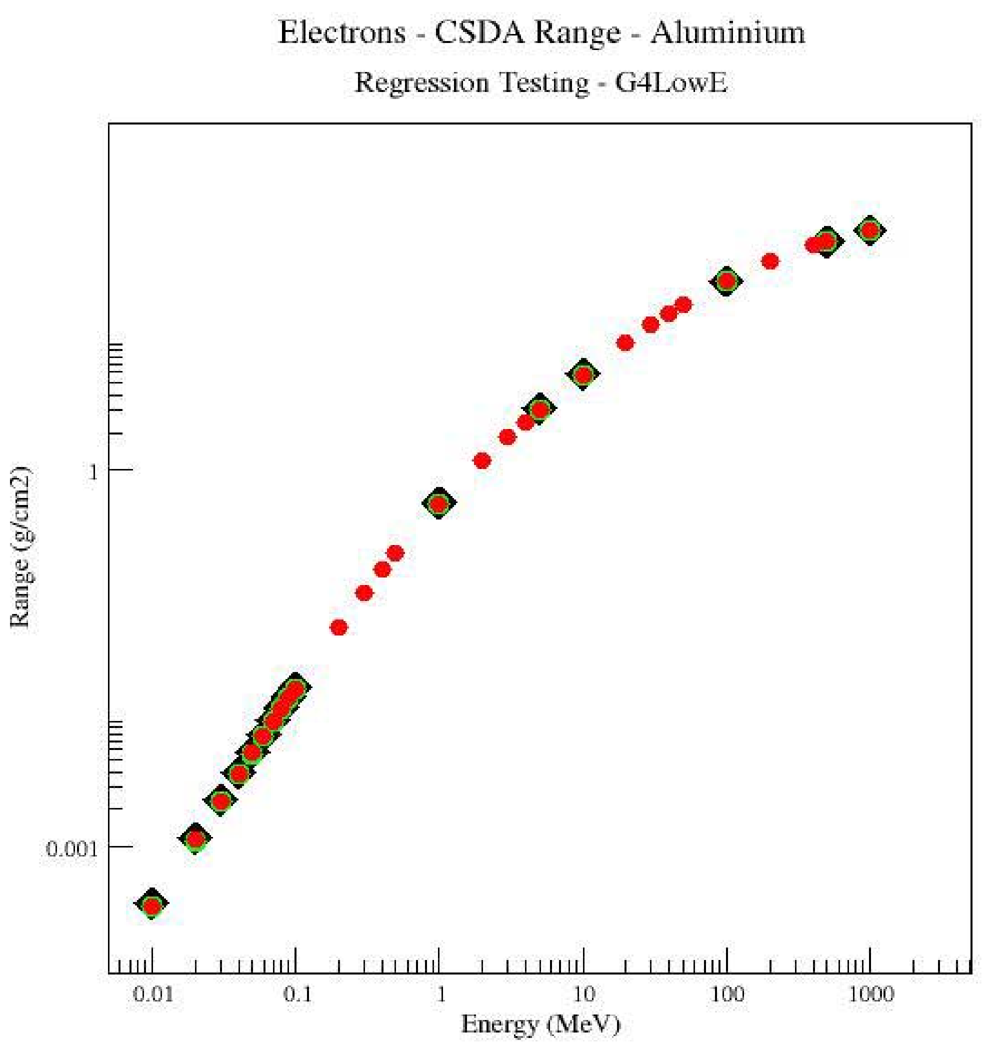


NIST-ESTAR

G4 Standard

G4 LowE

CSDA Range – Al –G4LowE



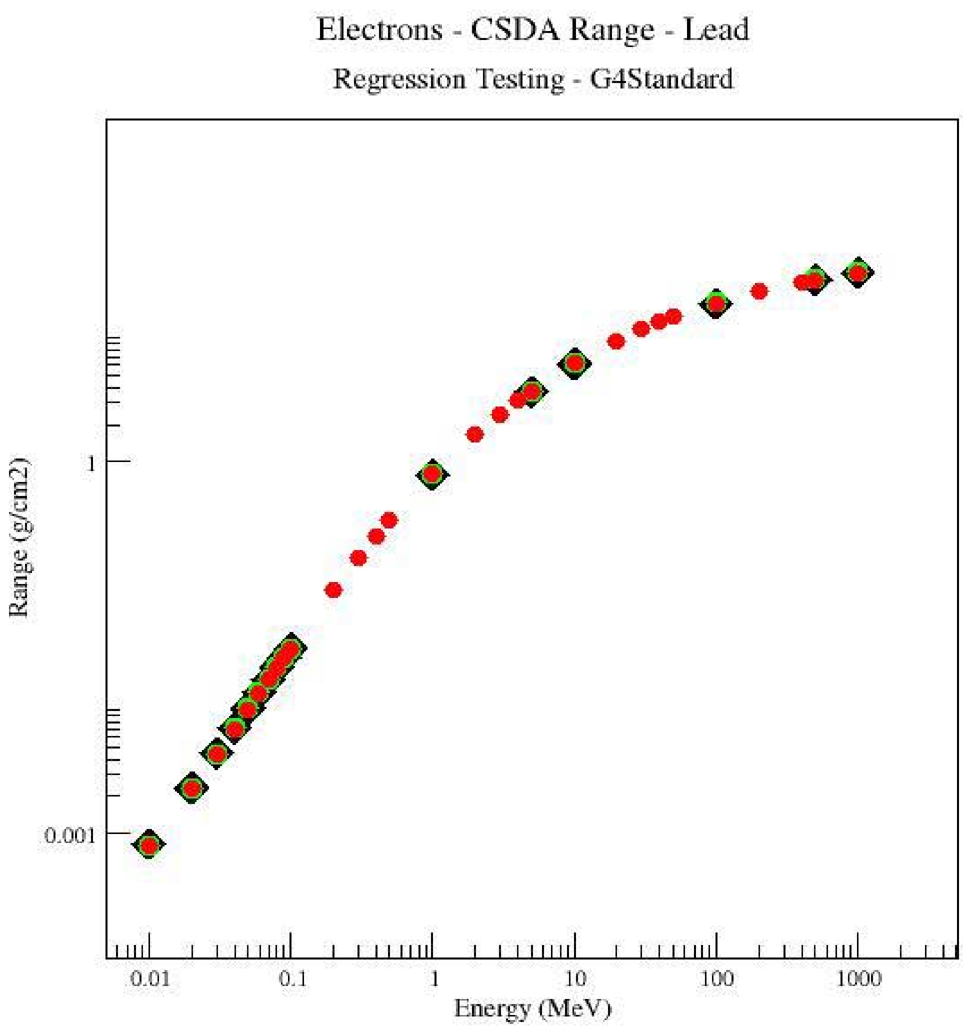
Regression testing

NIST-ESTAR

Geant4-05-00

Geant4-05-02

CSDA Range – Pb –G4Standard

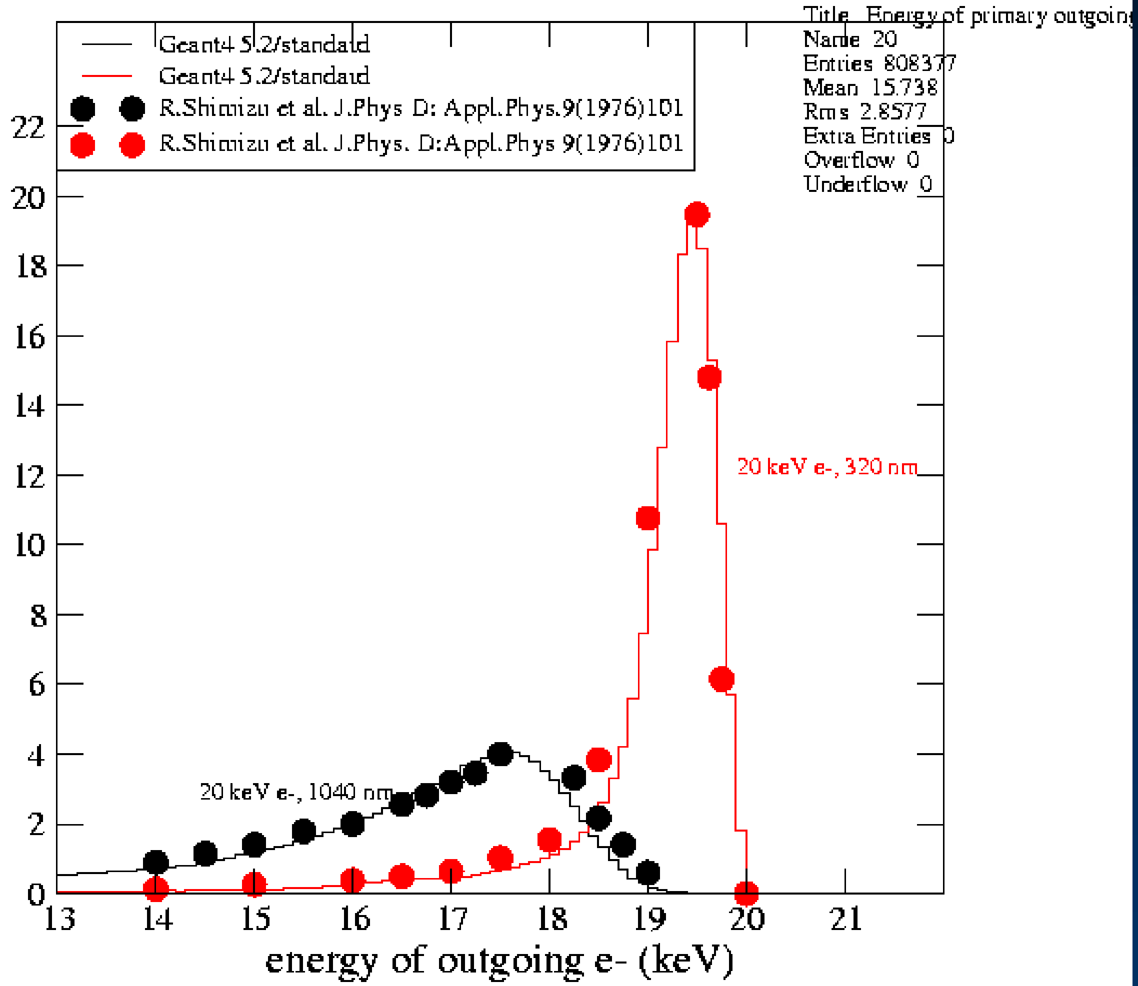


Regression testing

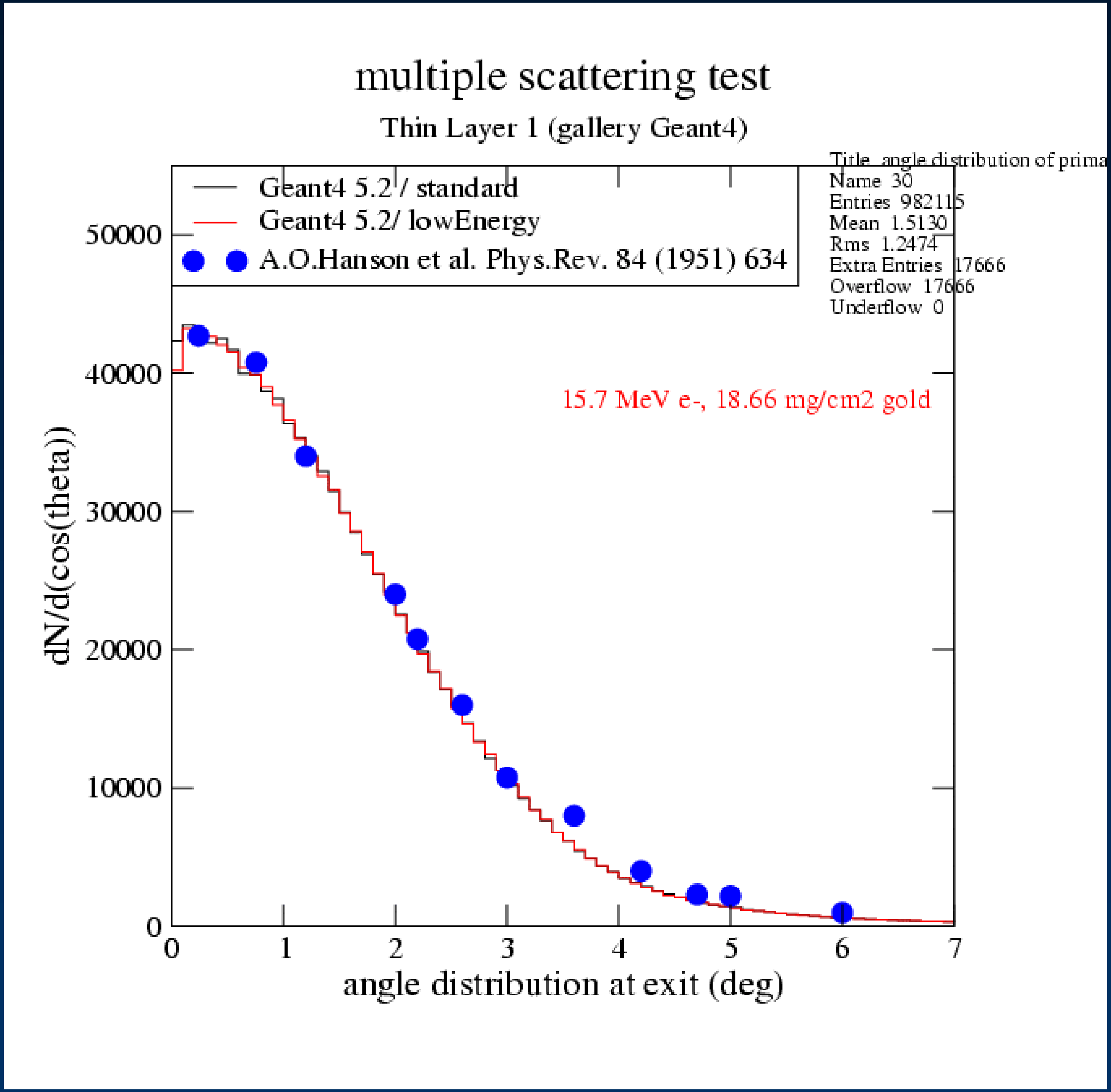
Test results

Transmission

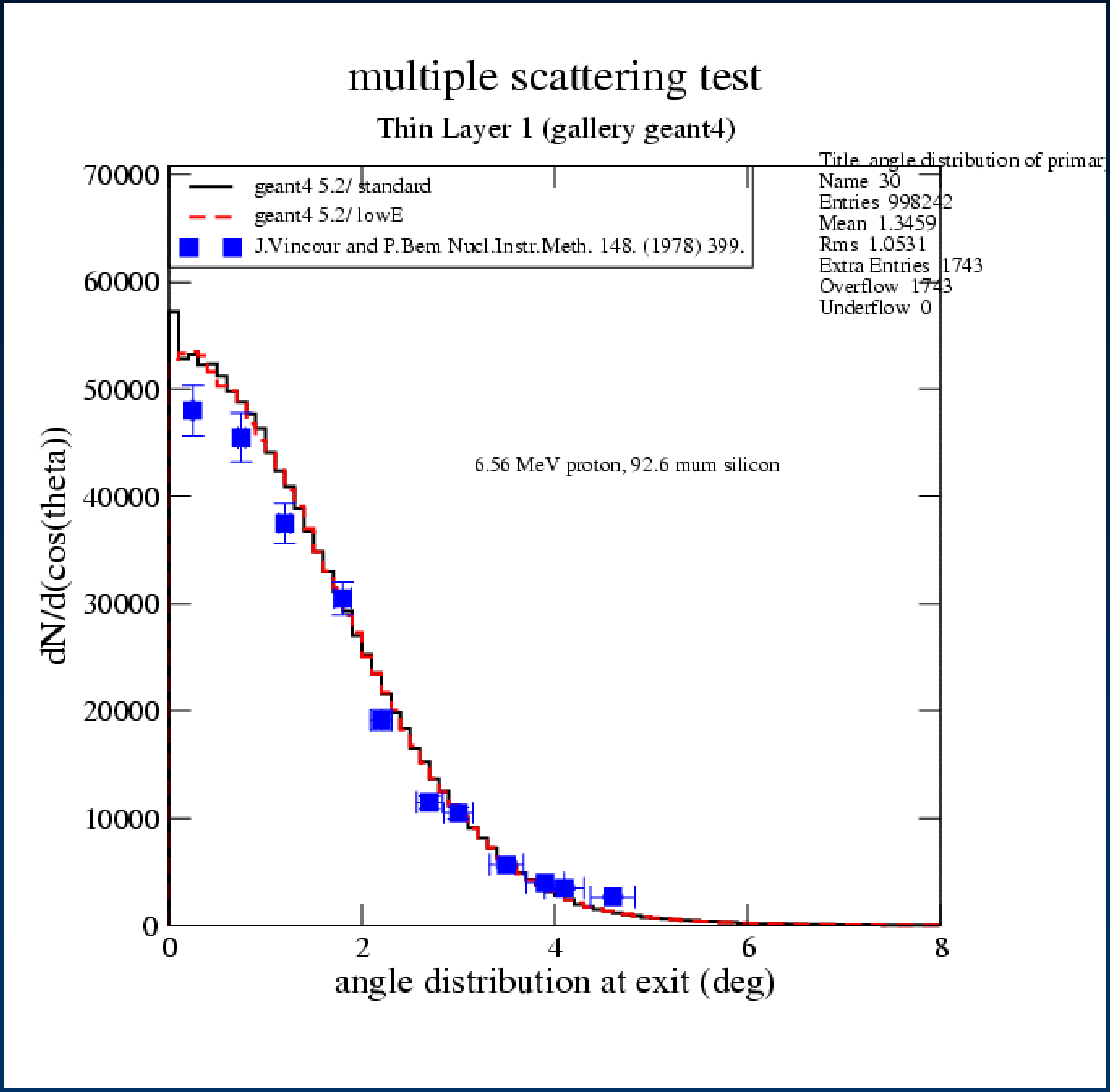
Energy distributions of transmitted e- on Al



Angular distribution of transmitted electrons



Angular distribution of transmitted protons



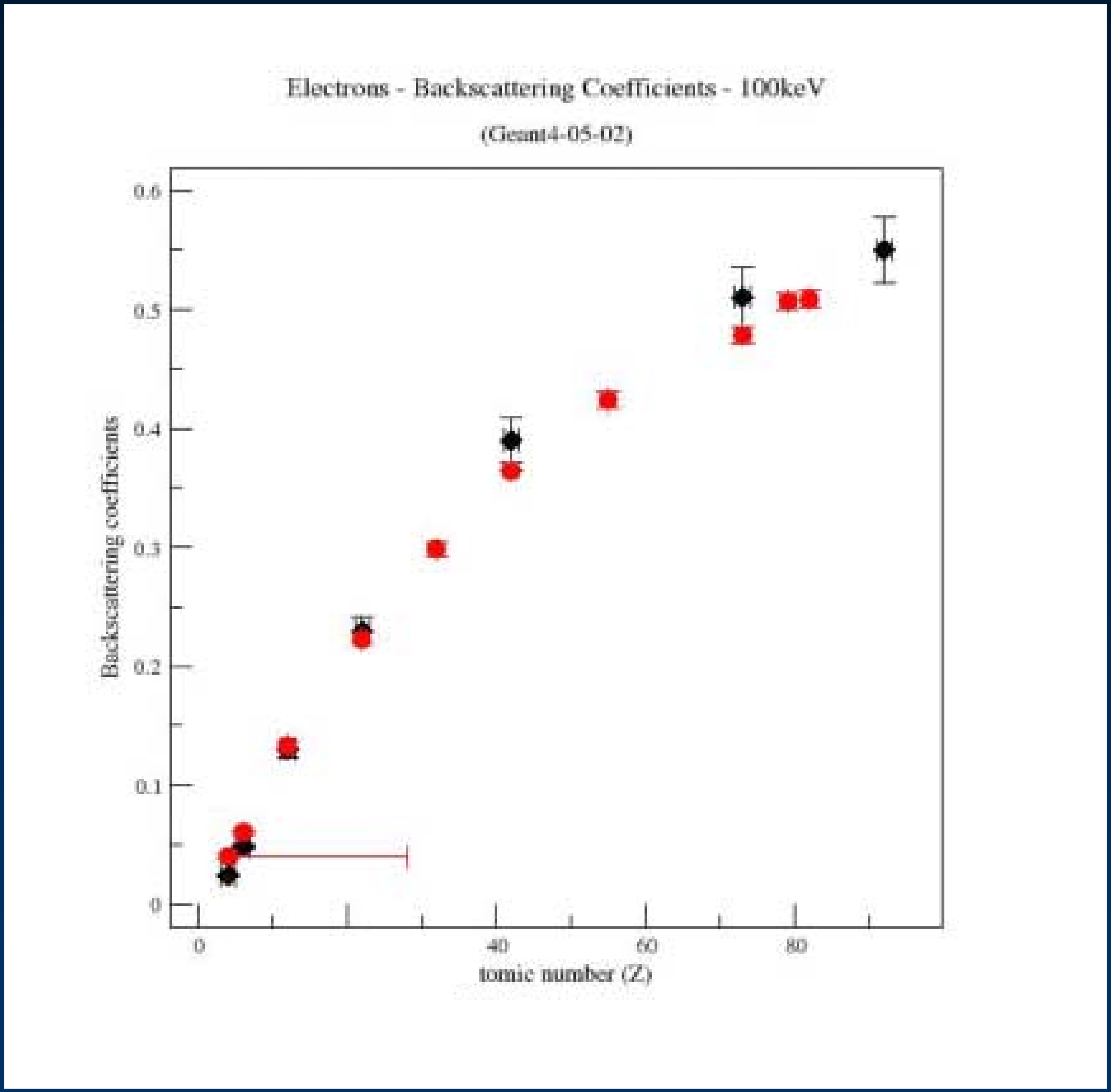
Test results

Backscattering for electrons and positrons

<u>Absorber Materials</u>:

Be, Al, Si, Ge, Fe, Mg, Ag, Au

Backscattering coefficient – E=100keV

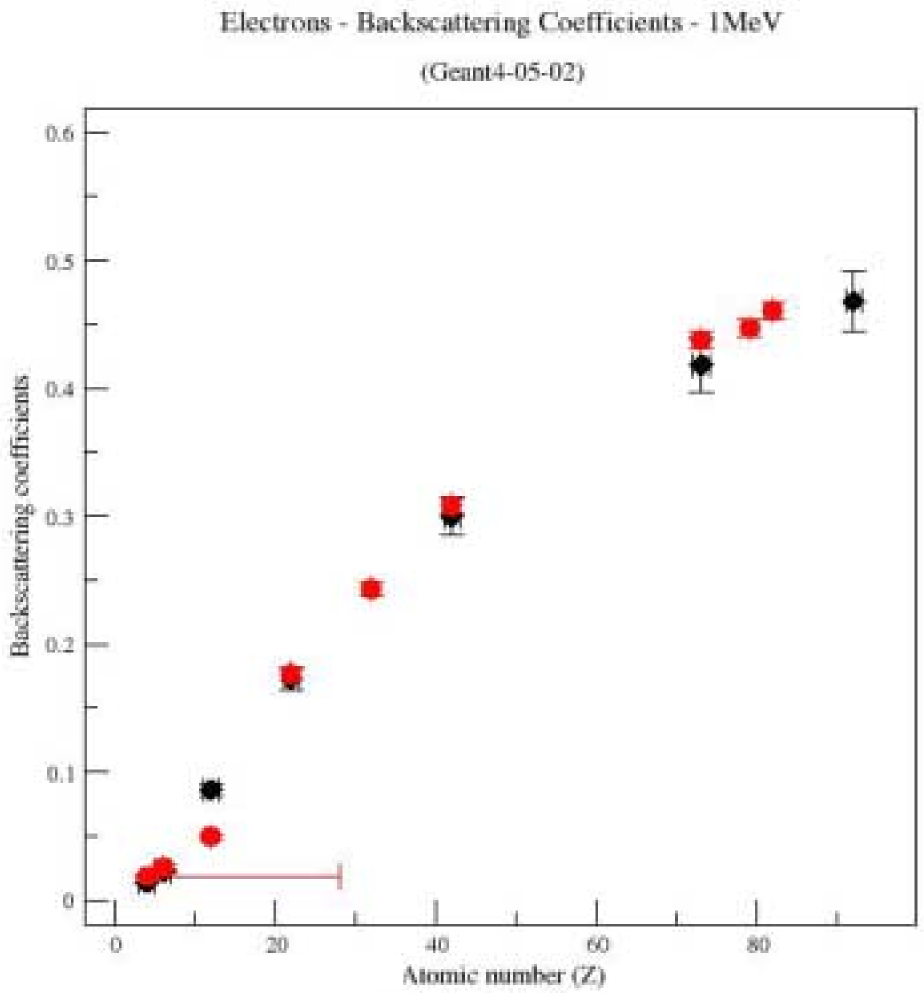


Angle of incidence (with respect to the normal to the sample surface) = 0°

Lockwood et al. (1981)

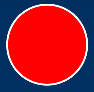
G4 LowE

Backscattering coefficient – E=1MeV



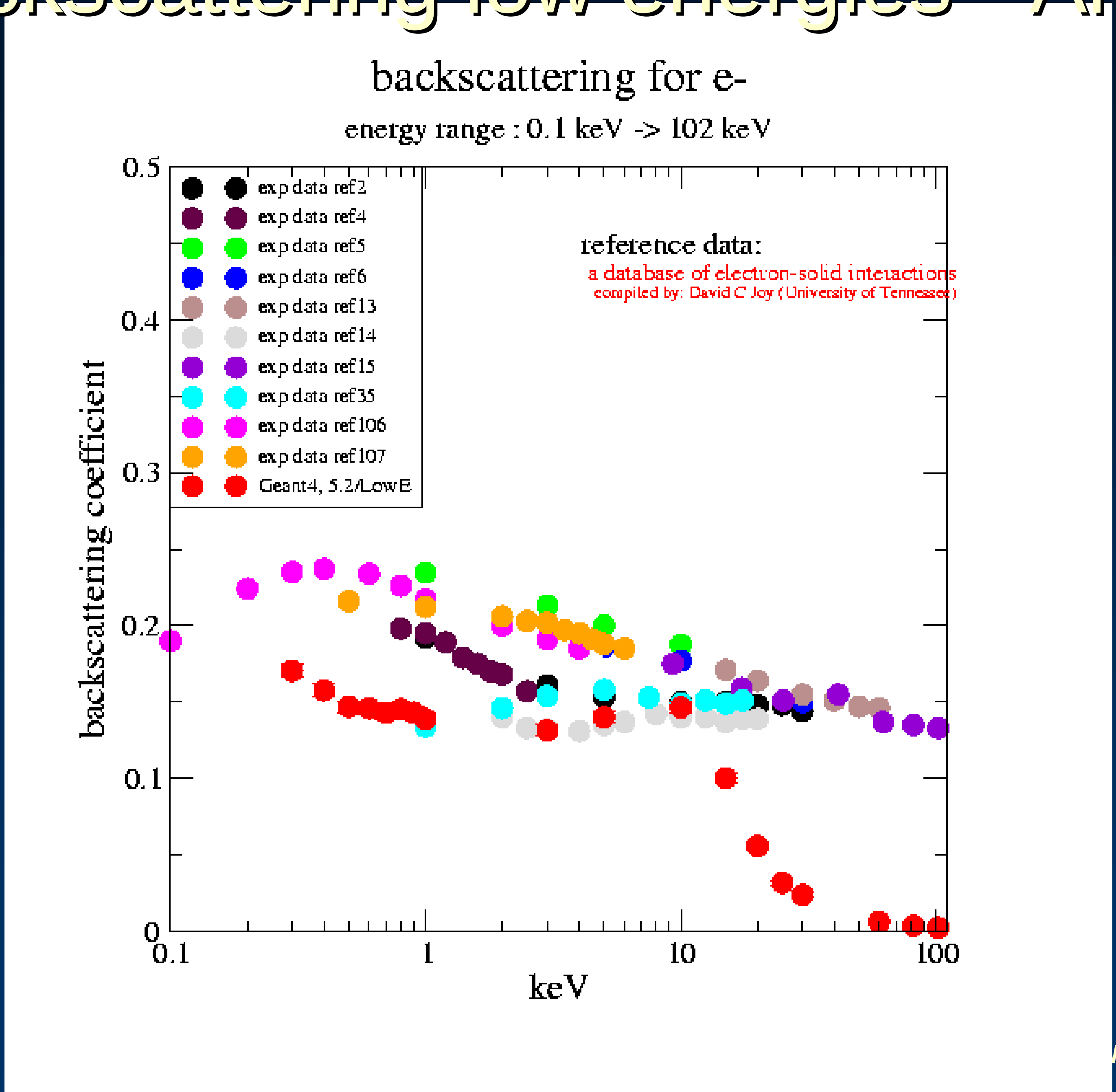
Angle of incidence (with respect to the normal to the sample surface)=0°

Lockwood et al. (1981)

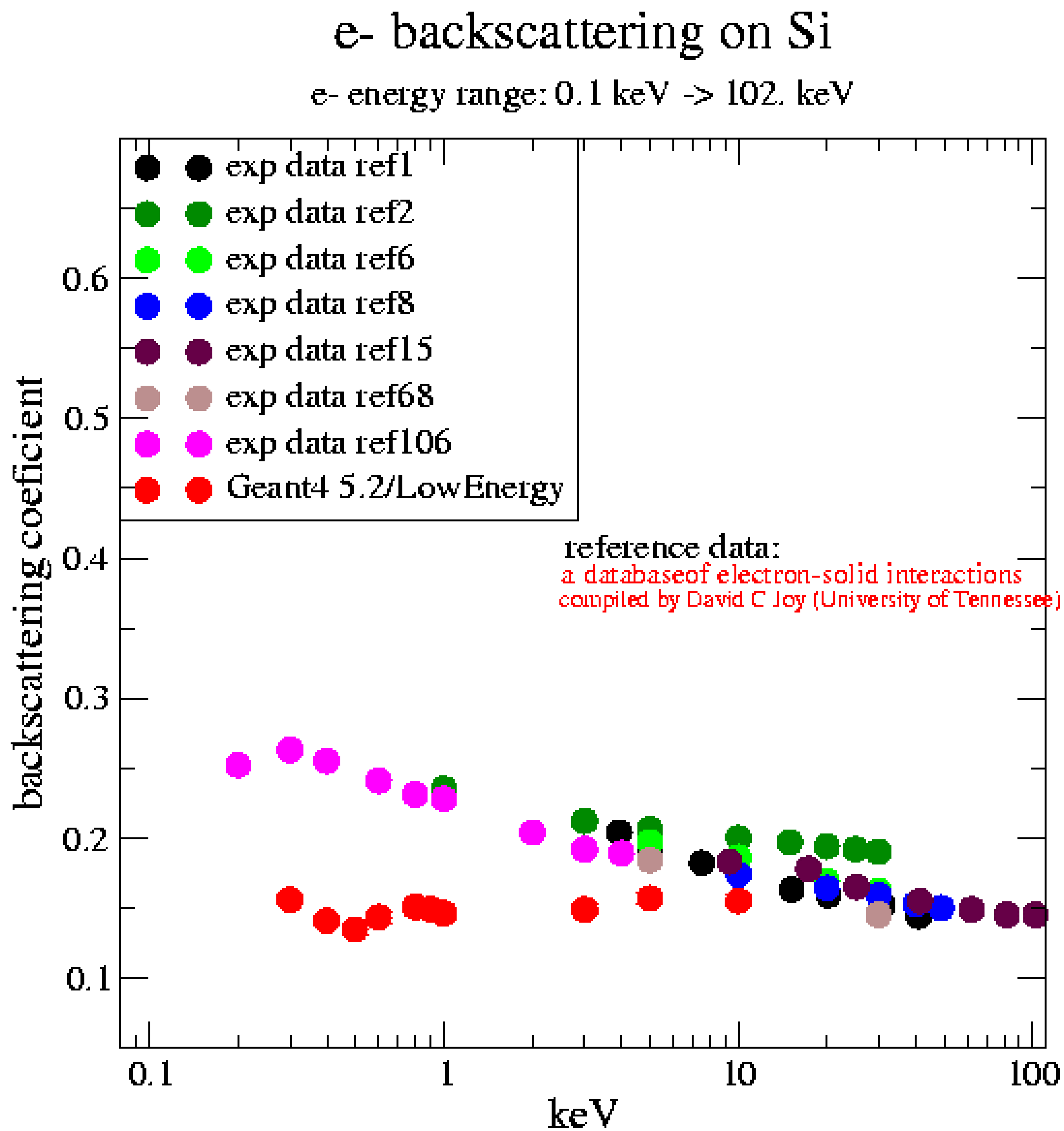


G4 LowE

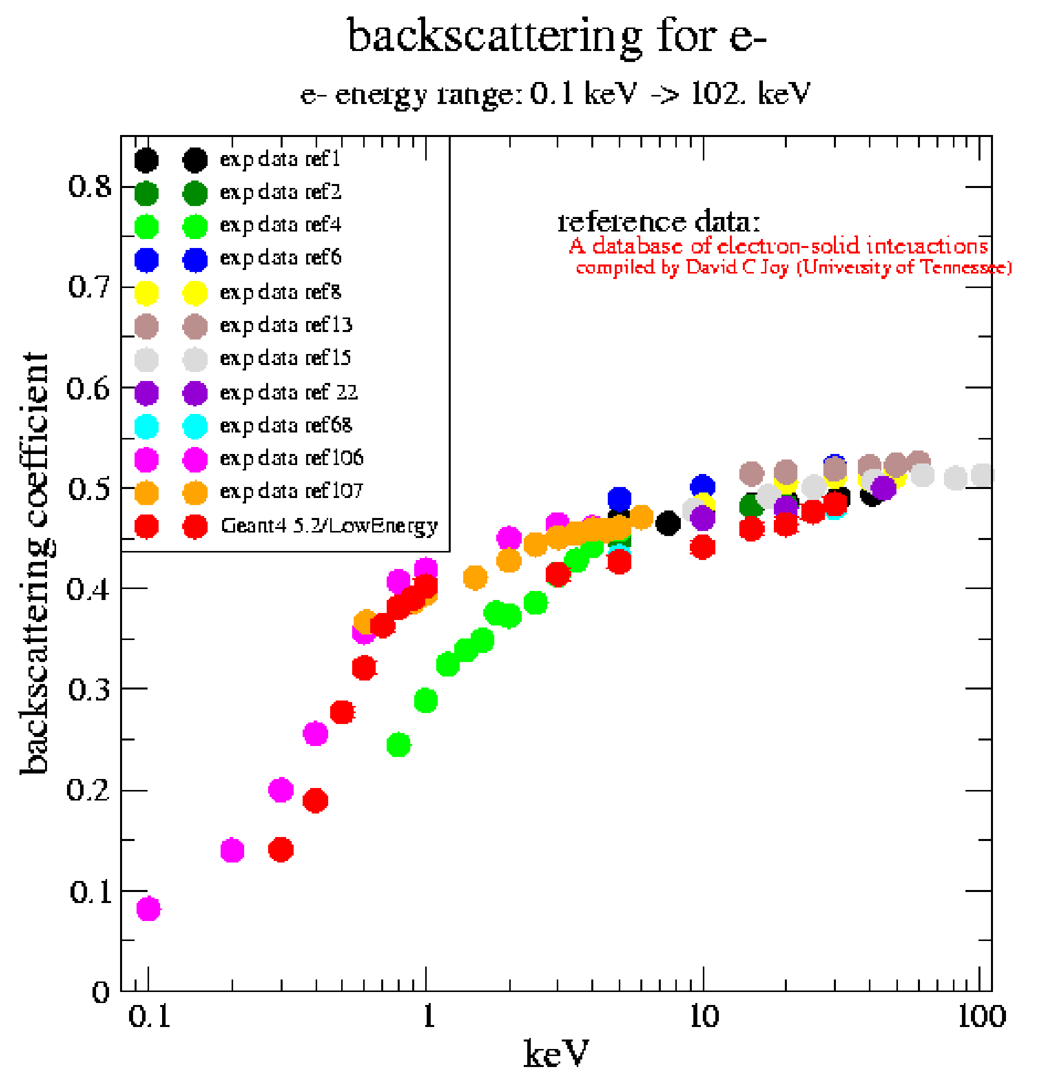
Backscattering low energies - Al



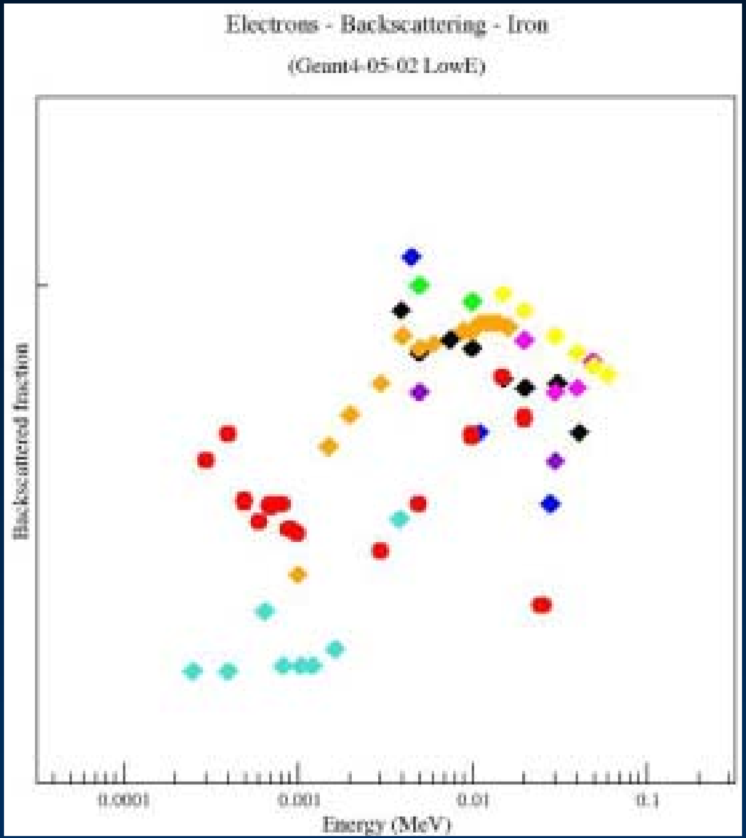
Backscattering low energies - Si



The problem of validation: finding reliable data



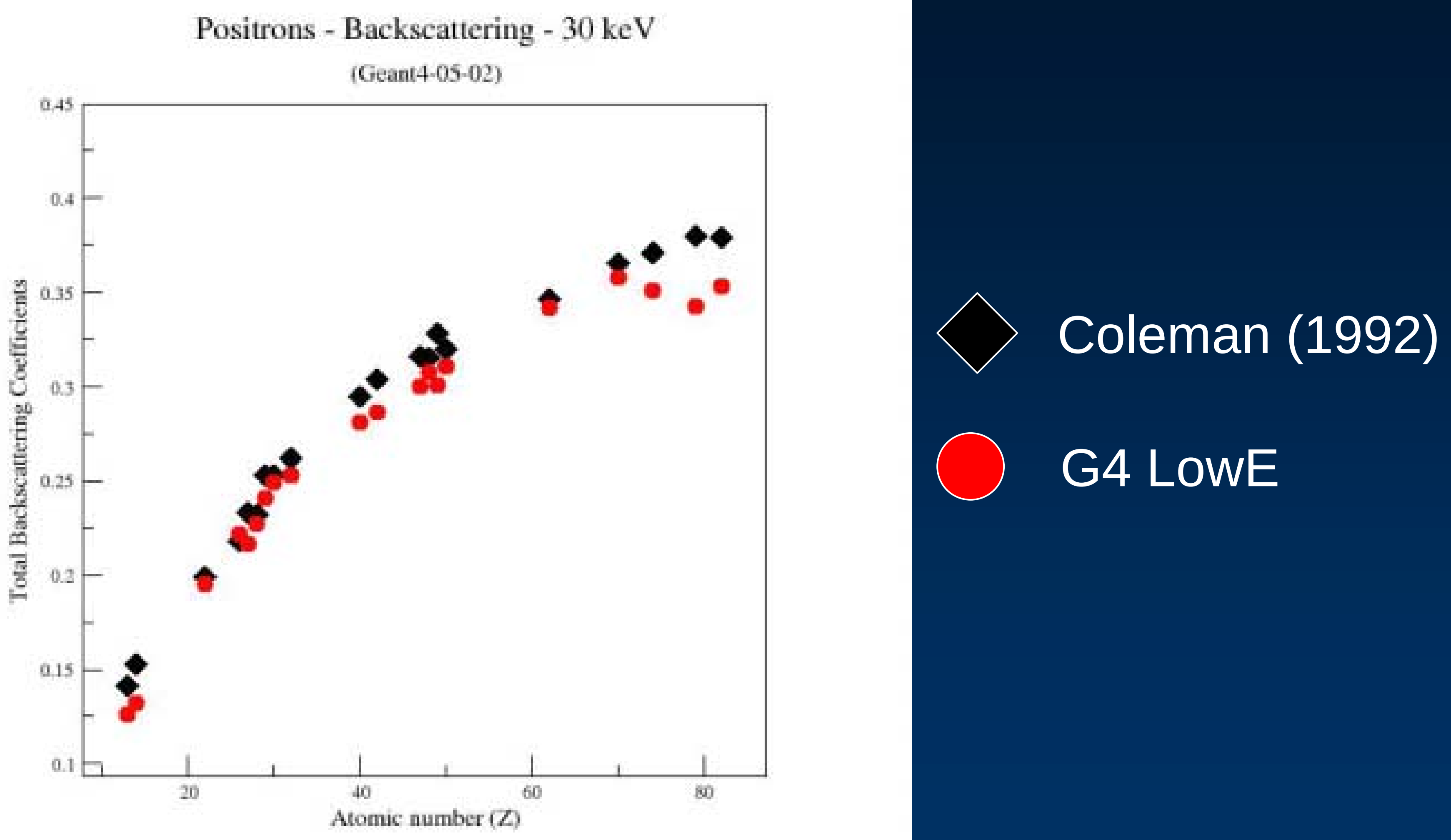
Backscattering low energies - Au

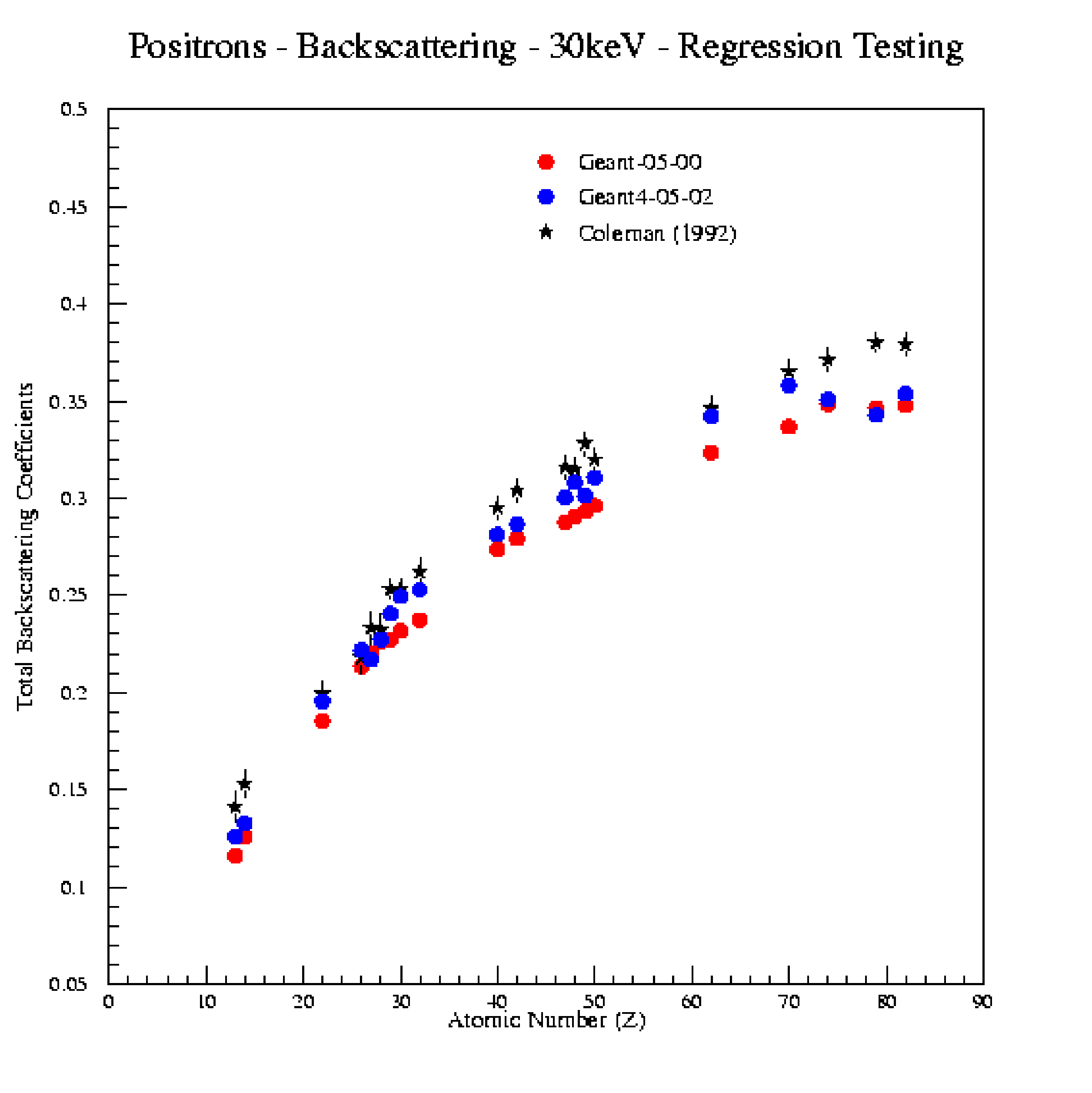


Note: Geant4 validation is not always easy

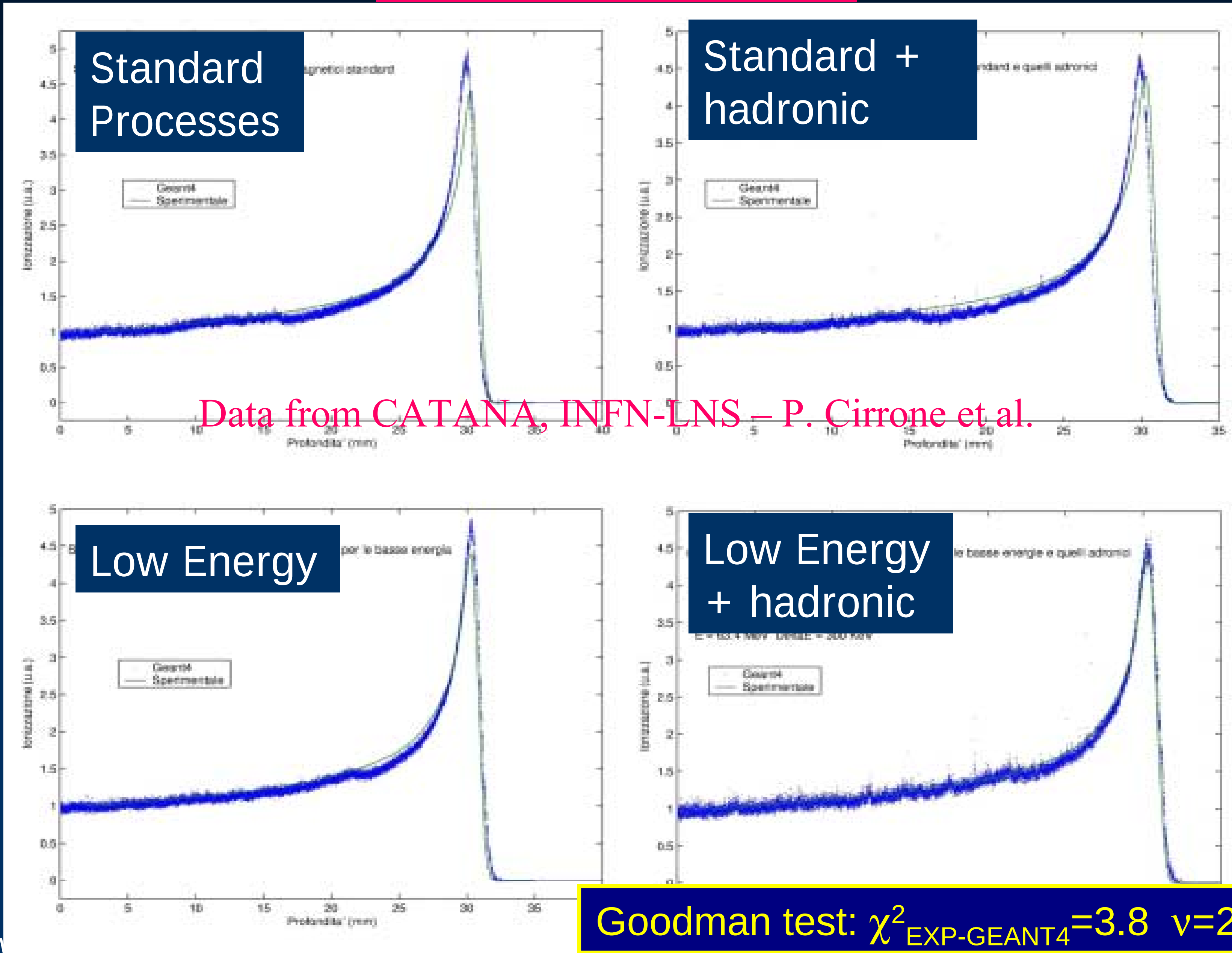
experimental data often exhibit large differences!

Backscattering coefficient – 30keV




Positrons - Backscattering - 30keV - Regression Testing
Geant-05-00
Geant4-05-02
Coleman (1992)
Total Backscattering Coefficients
Atomic Number (Z)
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0
10
20
30
40
50
60
70
80
90

Bragg peak, protons



Data from CATANA, INFN-LNS – P. Cirrone et al.

Goodman test: $\chi^2_{EXP-GEANT4}=3.8$ $\nu=2$ p=n.s.

Contributions from users

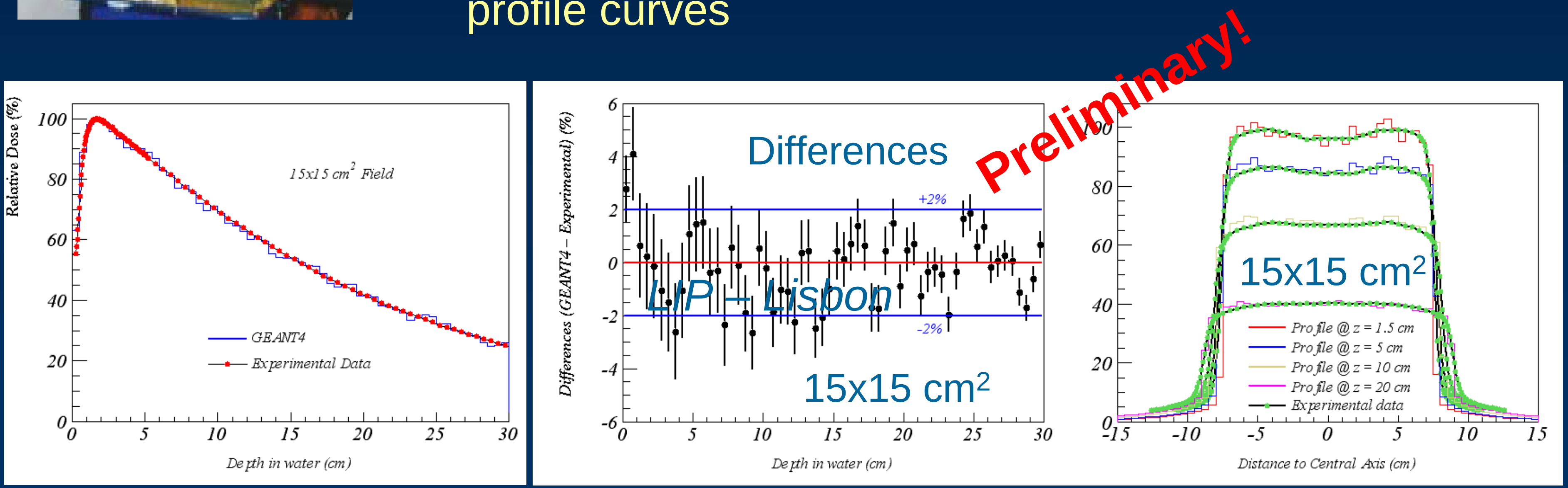
Contribution from users

- Many valuable contributions to the validation of LowE physics from users all over the world
  - excellent relationship with our user community
- A small sample in the next slides
  - no time to show all!
- Feel free to contact us!

Homogeneous Phantom

P. Rodrigues, A. Trindade, L.Peralta, J. Varela, LIP

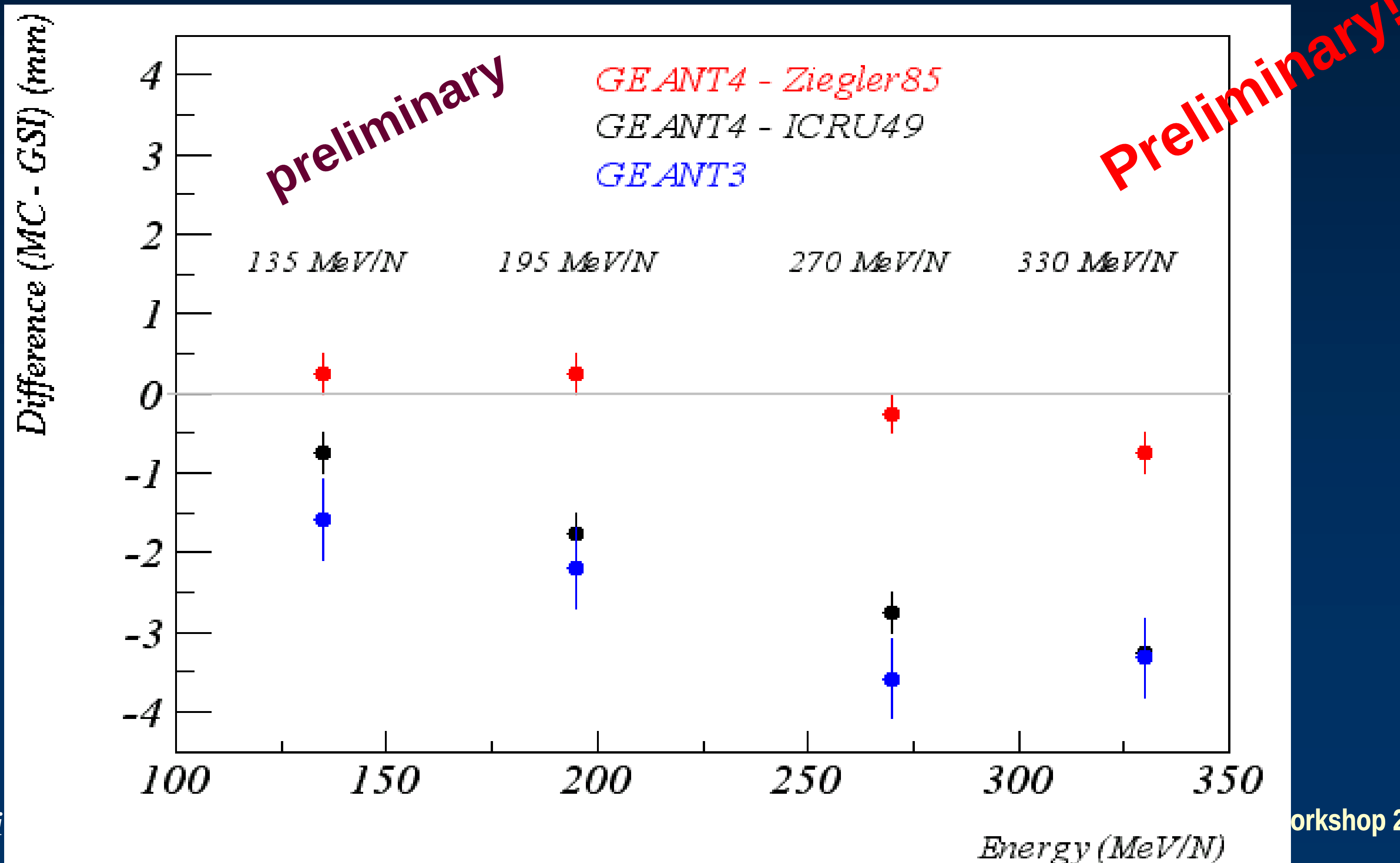
- Simulation of photon beams produced by a Siemens Mevatron KD2 clinical linear accelerator
- Phase-space distributions interface with GEANT4
- Validation against experimental data: depth dose and profile curves



Dose Calculations with 12C

P. Rodrigues, A. Trindade, L.Peralta, J. Varela, LIP

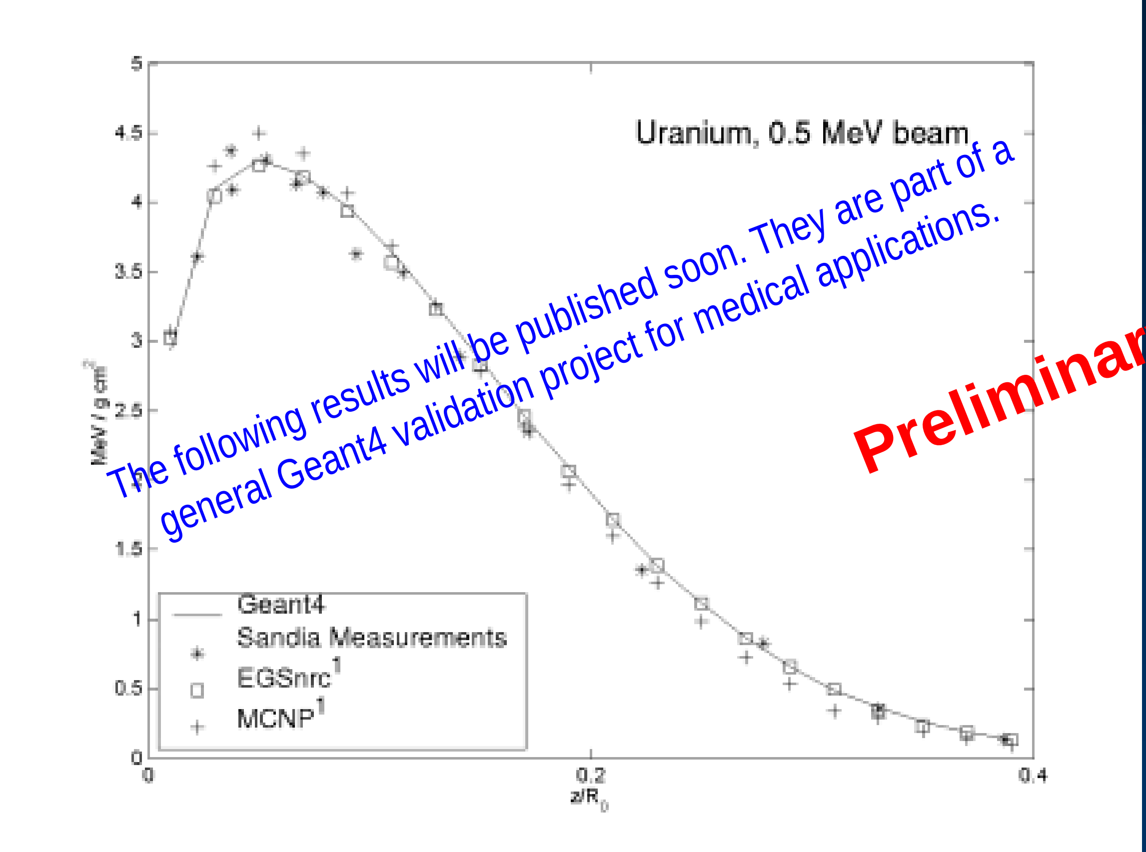
- Bragg peak localization calculated with GEANT4 (stopping powers from ICRU49 and Ziegler85) and GEANT3 in a water phantom
- Comparison with GSI data



Uranium irradiated by electron beam

Jean-Francois Carrier, Louis Archambault, Rene Roy and Luc Beaulieu

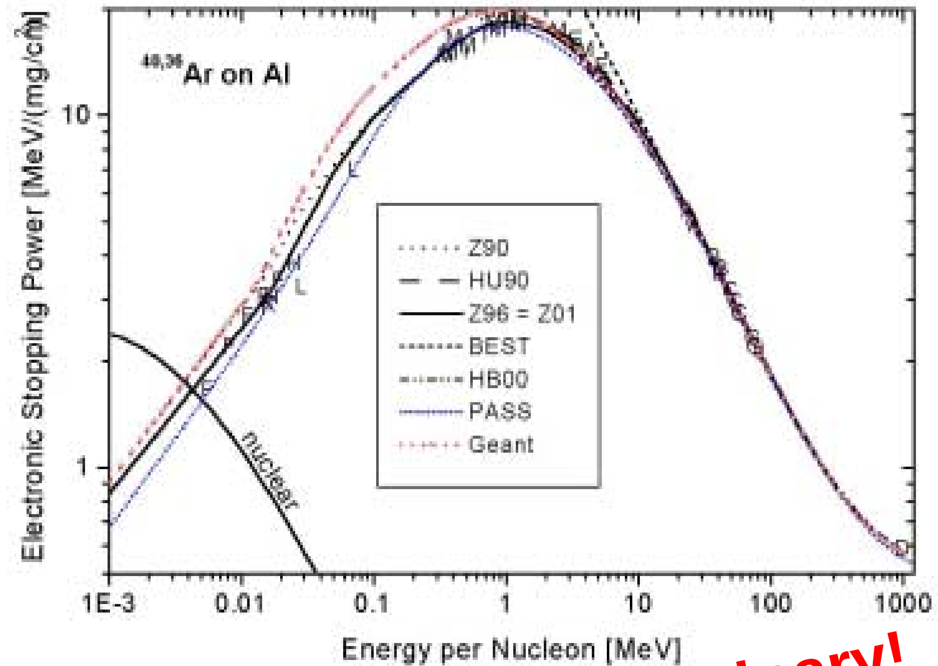
Service de radio-oncologie, Hotel-Dieu de Quebec, Quebec, Canada
Departement de physique, Universite Laval, Quebec, Canada



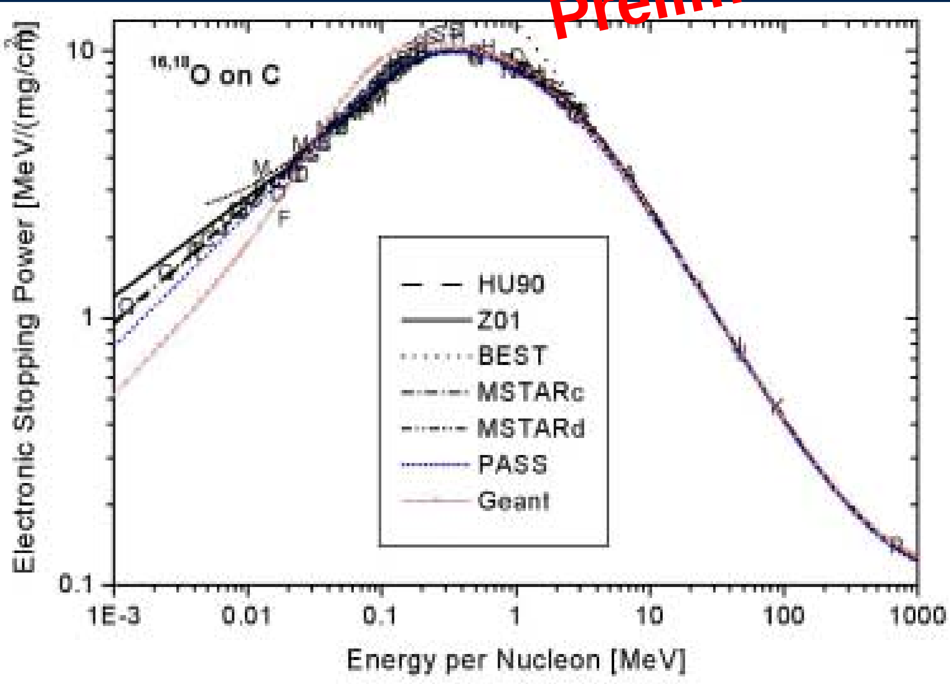
Depth-dose curve for a semi-infinite uranium slab irradiated by a 0.5 MeV broad parallel electron beam

[1]Chibani O and Li X A, Med. Phys. 29 (5), May 2002

Ions



Geant4-LowE reproduces the right side of the distribution precisely, but about 10-20% discrepancy is observed at lower energies



H. Paul, Univ. Linz

Conclusions

To learn more

- Geant4 Physics Reference Manual
- Application Developer Guide

- http://www.ge.infn.it/geant4/lowE

Low Energy Electromagnetic Physics

- Stéphane Chauvie
- Stefania Donadio
- Susanna Guatelli
- Vladimir Ivanchenko
- Francesco Longo
- Alfonso Mantero
- Barbara Mascialino
- Petteri Nieminen
- Luciano Pandola
- Sandra Parlati
- Luis Peralta
- Andreas Pfeiffer
- Maria Grazia Pia
- Pedro Rodrigues
- Simona Saliceti
- Andreia Trindade
- *Paolo Viarengo*

⟷

Advanced Examples

- Stefano Agostinelli
- Henrique Araujo
- Pablo Cirrone
- Giacomo Cuttone
- Maria Catarina Espirito Santo
- Franca Foppiano
- Stefania Garelli
- Patricia Goncalves
- Alex Howard
- Ana Keating
- Susanne Larsson
- Jakub Moscicki
- Michela Piergentili
- Giovanni Santin
- Bernardo Tome