Outlook
Ongoing developments in PENELOPE

F. Salvat-Pujol

On behalf of the PENELOPE team

OMA School on Monte Carlo simulations
(of radiation transport)

Nov 10, 2017

Particularities of the PENELOPE ecosystem

- Committed to e^-/e^+, photons. ~100 eV < E < 1 GeV.

- Development team (averaged from ~1987-2017):

F. Salvat,

J.M. Fernández-Varea, J. Sempau, (X. Llovet)

*Departament d'Estructura i Constituents de la Matèria****

UNIVERSITAT DE BARCELONA

- Corridor: expertise in atomic/nuclear physics, numerically inclined

- Most differential cross sections calculated in-house.

- Often resulting in standard reference databases.

Plan for this talk

1) Elastic scattering of electrons and positrons.
ELSEPA (2005) → ICRU77 (2007) → NIST SRD64 (2016).

2) Cross sections for atomic inner-shell ionization by e-/e+ impact.
Bote & Salvat (2008) → J Phys Chem Ref Dat (2014) → NIST164 (2015).

3) Photoelectric absorption: Sabbatucci & Salvat (2016).

4) PENH: proton transport
Class II, EM interactions only, elastic scattering (screened point nucleus), nuclear elastic scattering and nuclear recoil effects (dev).

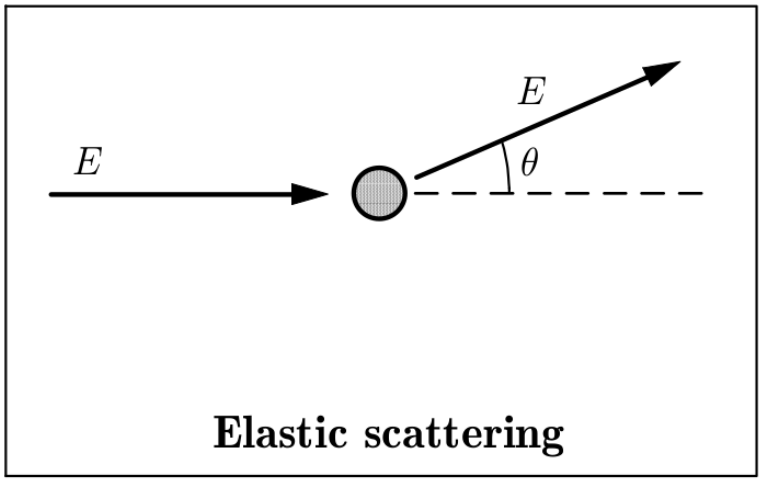
5) Radioactive sources (Garcia-Toraño 2017)

6) PenGeom viewer in Java

Slightly heavy, but effort made to pass the main points leaving technicalities aside.

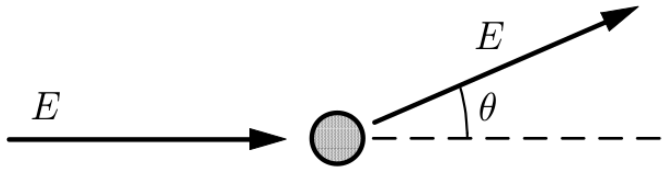
1) Elastic scattering of e^-/e^+ on atoms

1) Elastic scattering of e^-/e^+



- Reminder: deflection (change of direction) of e^-/e^+ as result of interaction with atomic potential.
- In many MC codes: screened Rutherford diff xs (additional corrections: screening, spin-relativ effects).
- Strictly: solve scattering problem (overlap between solutions of Schroedinger eq for this problem, e.g. plane waves).
- A bit better: plane waves distorted by atomic potential.

Even more realistic



Elastic scattering

Available online at www.sciencedirect.com
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Computer Physics Communications

ELSEVIER

Computer Physics Communications 165 (2005) 157–190

www.elsevier.com/locate/cpc

ELSEPA—Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules ☆

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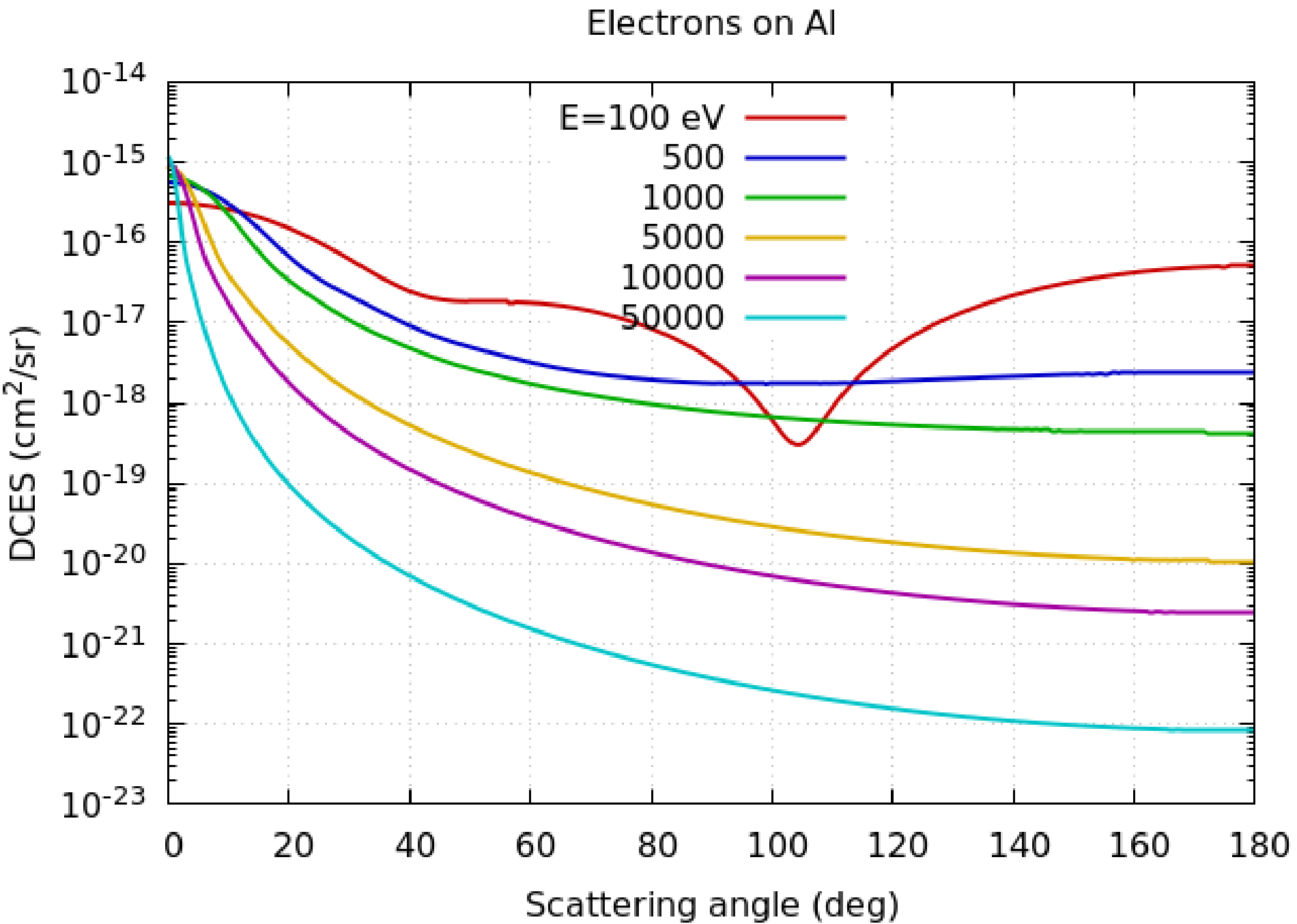
[b] *Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland*
[c] *Surface and Microanalysis Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8370, USA*

Received 19 March 2004

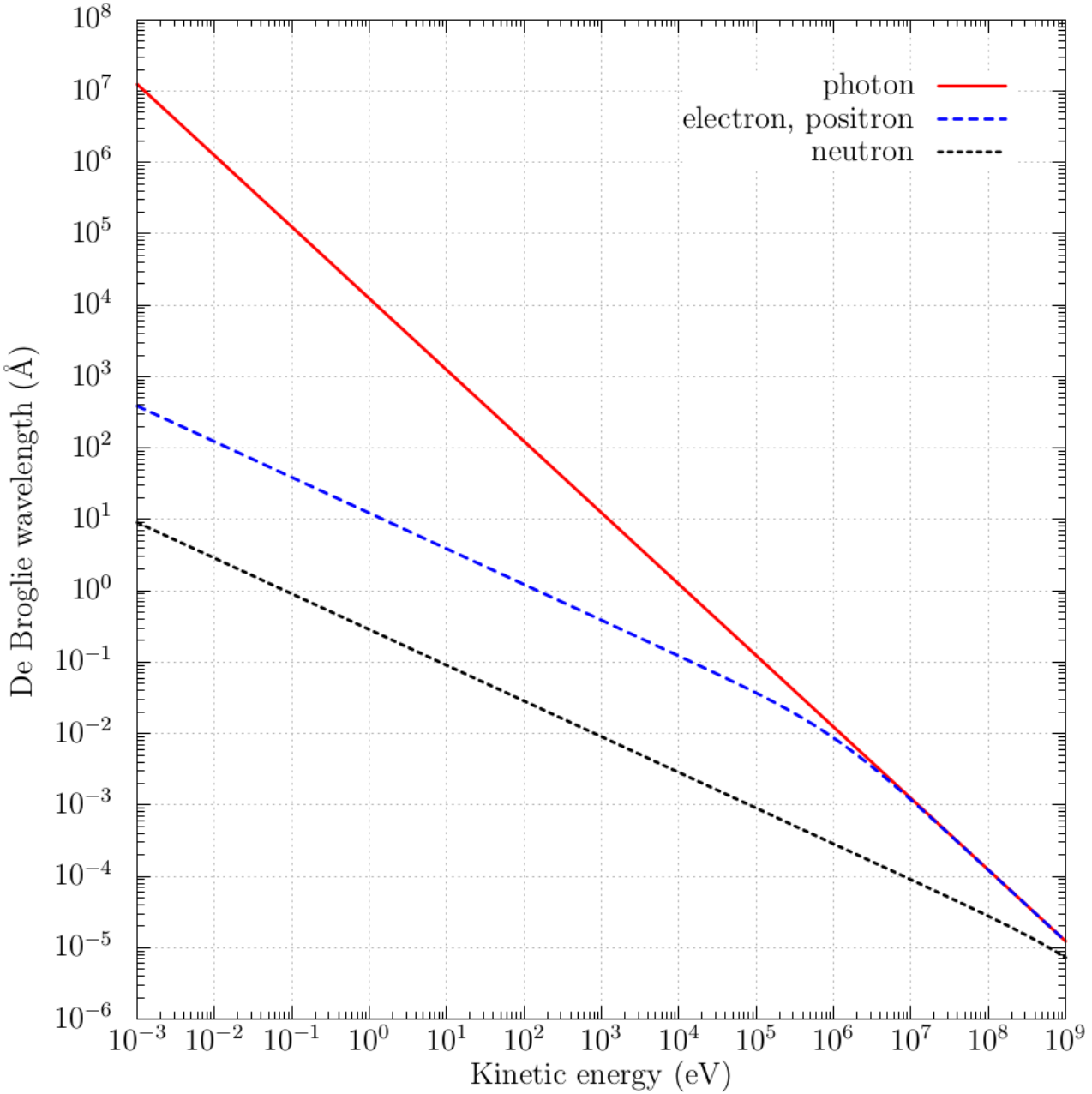
Note the direct acceptance…

Screened Rutherford is fine at moderate and high ene



Why the structure at low E?

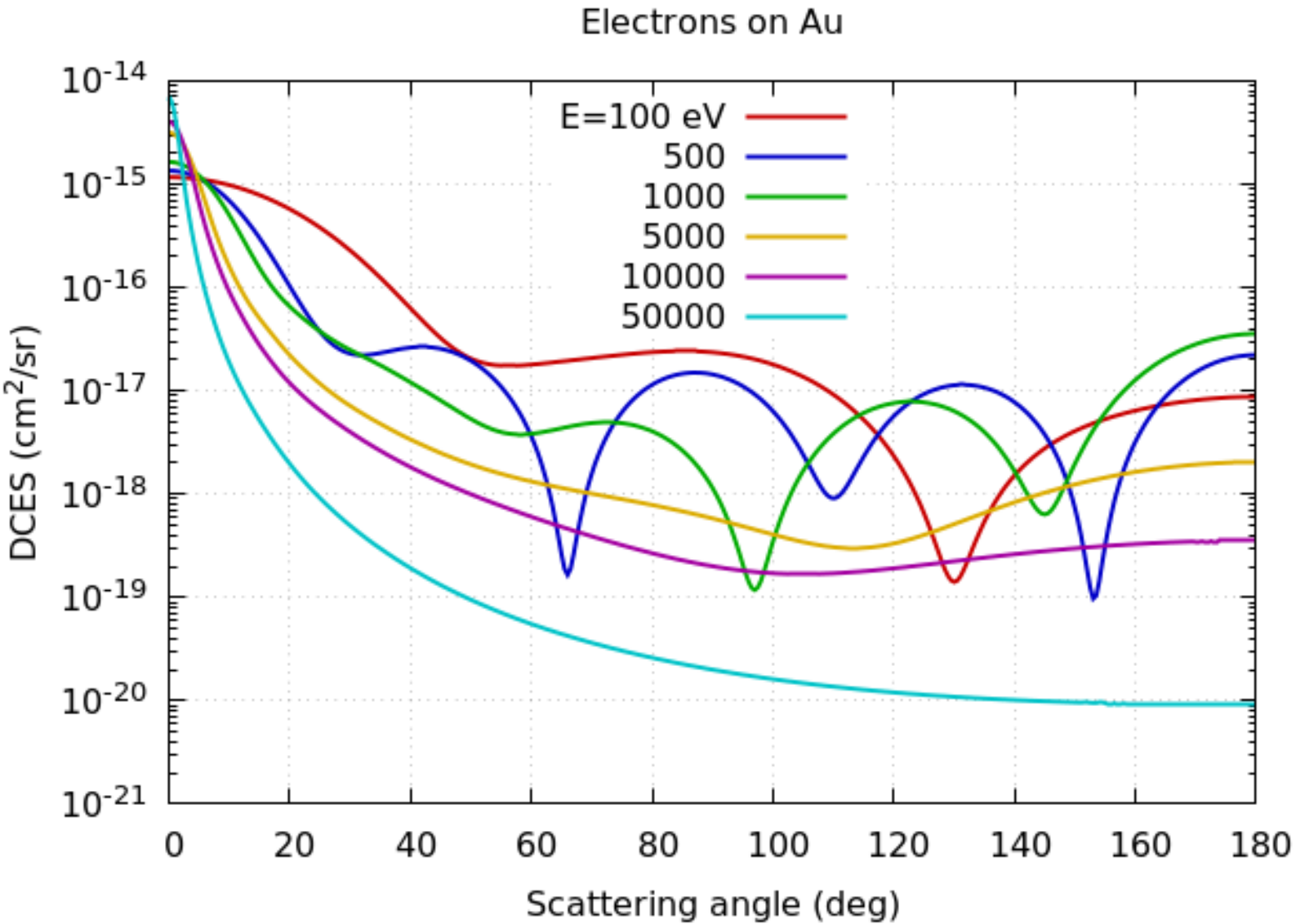
The de-Broglie wavelength becomes comparable to atomic radius
No longer particle description, wave nature → diffraction effects (!) → structure of minima
The higher Z, the more complicated is the atomic structure, the richer the structure



Elastic scattering on heavy elements

Structure more visible at large scattering angles (small impact parameters).
Intoxicated gentleman simile:

large impact parameters (does not probe e- dens) ↔ small scattering angles
small impact parameters (probes e- density) ↔ large scattering angles



Volume 7 No 1 2007 ISSN 1473-6691

Journal of the ICRU

ICRU REPORT 77

Elastic Scattering of Electrons and Positrons

Cross check with Martin Berger (<2004)
Comparison with experimental data

Comparison with experiment

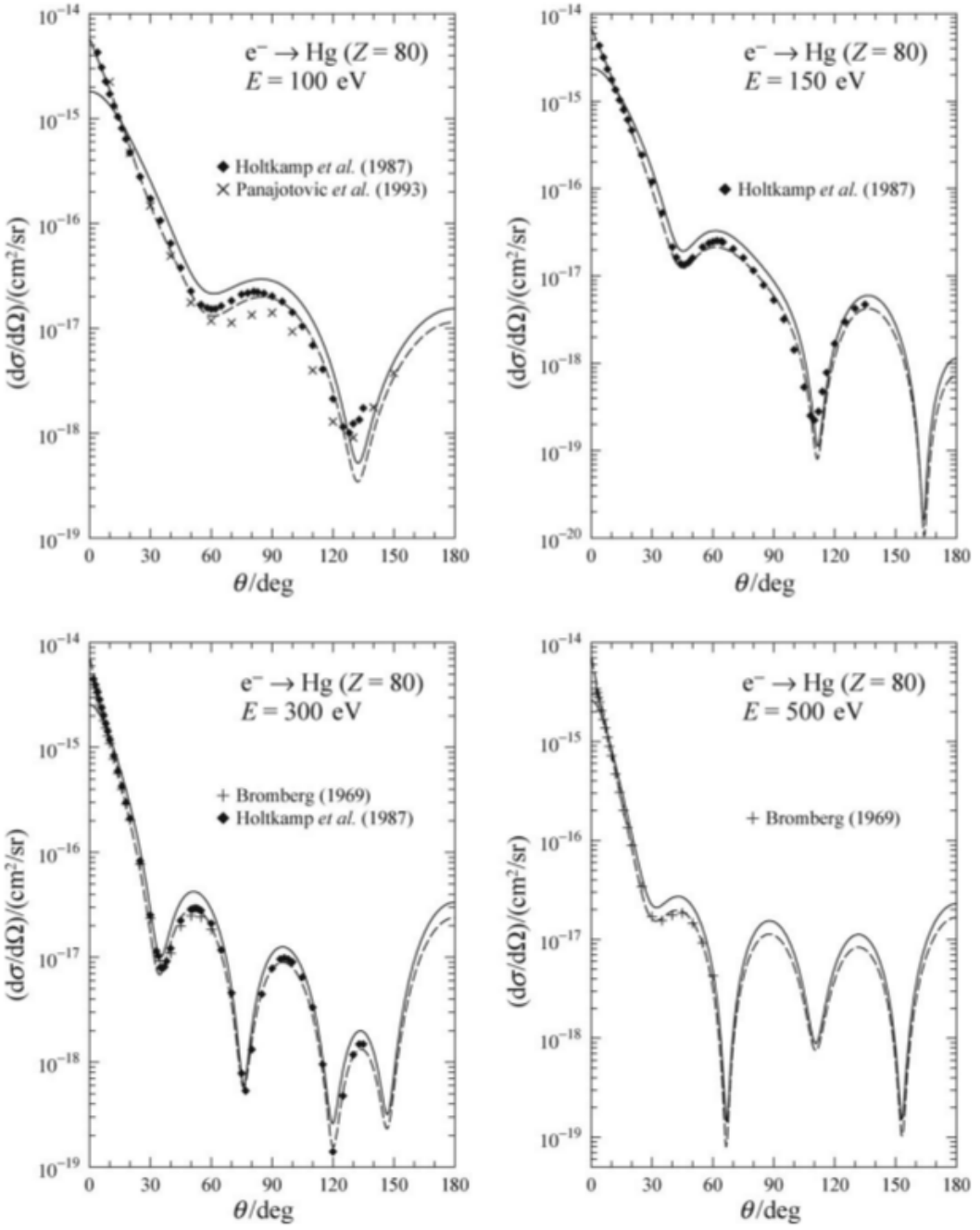


Figure 5.7. Differential cross-sections for elastic scattering of electrons by mercury atoms. Symbols represent experimental data from the quoted references. The solid curves represent DCSs calculated from the F–DF–FM potential. Dashed curves are results from calculations with the F–DF–FM–LDA–A optical model potential, with the default values of the potential parameters. Adapted from Salvat (2003).

NIST Electron Elastic-Scattering Cross-Section Database - Chromium

Home - Internati | NIST Electron El

Secure | https://srdata.nist.gov/srd64/

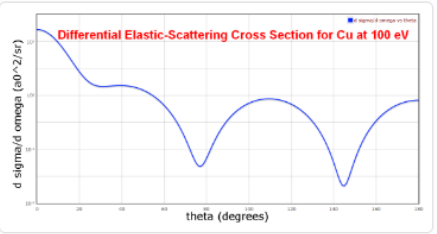
National Institute of Standards and Technology
U.S. Department of Commerce

NIST Electron Elastic-Scattering Cross-Section Database, SRD 64

Elastic-Scattering Cross Sections | Transport Cross Sections | Search | More Options

NIST Standard Reference Database (SRD) 64
NIST Electron Elastic-Scattering Cross-Section Database

Version 4.0



Data Provided By

Francesc Salvat, Universitat de Barcelona
Facultat de Fisica, Barcelona, Spain

Aleksander Jablonski, Institute of Physical Chemistry
Polish Academy of Sciences, Warsaw, Poland
and
Cedric J. Powell
National Institute of Standards and Technology, USA

Software Developed By

Angela Y. Lee, Aleksander Jablonski, and Francesc Salvat

Access the Database

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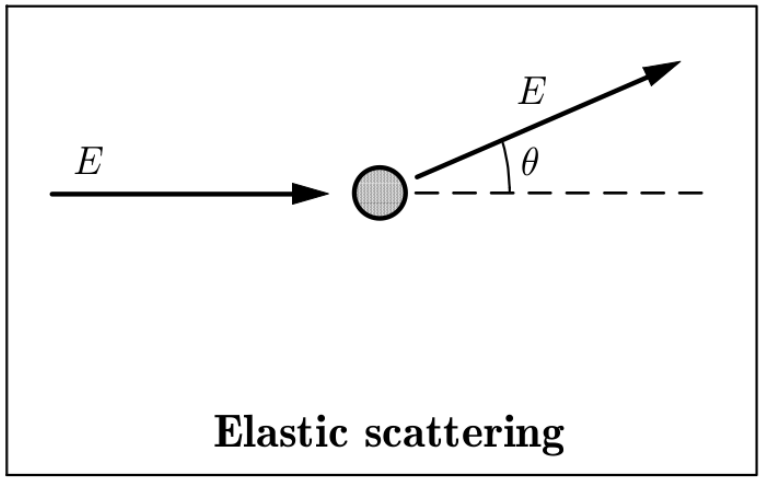
Introduction:

Theoretical description of electron transport in solids is important in radiation physics, electron lithography, electron-probe microanalysis, analytical

Date created: September 1, 2015 | Last updated: September 15, 2016 | Contact: data@nist.gov

Absorption



Experimentally: some electrons lost from elastic channel

Accounted by absorption term in potential

BUT

In PENELOPE: xs without absorption because inelastic collisions treated explicitly

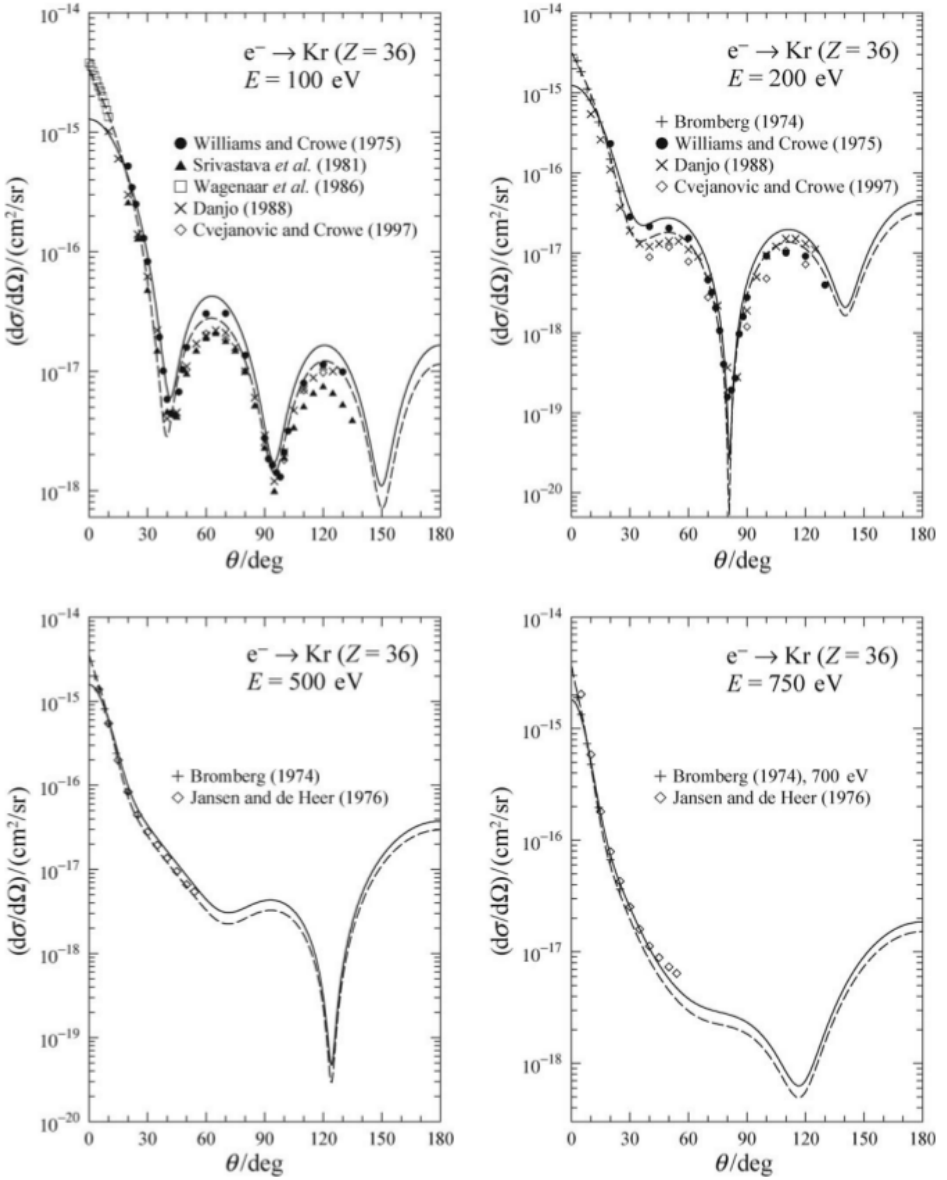
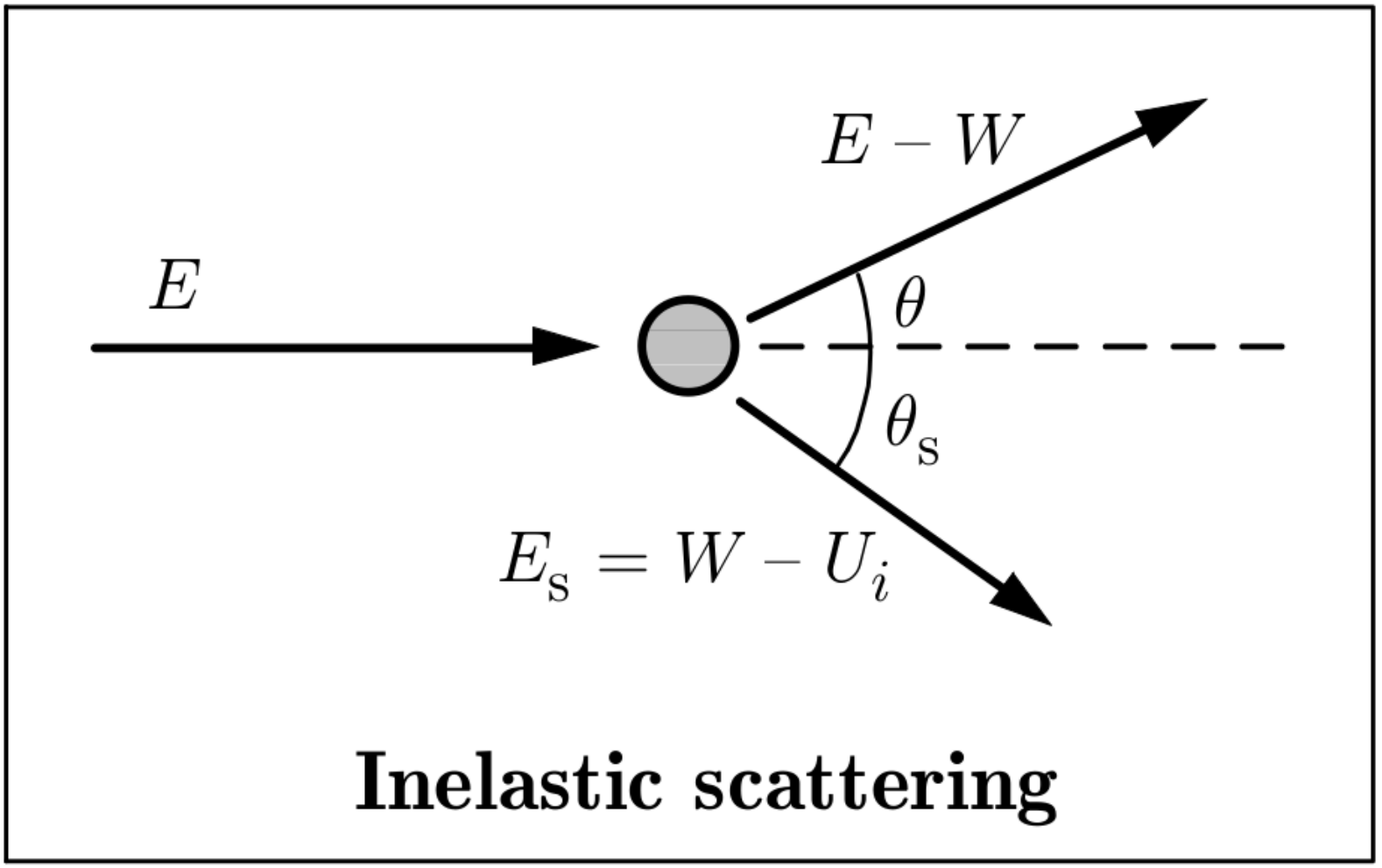
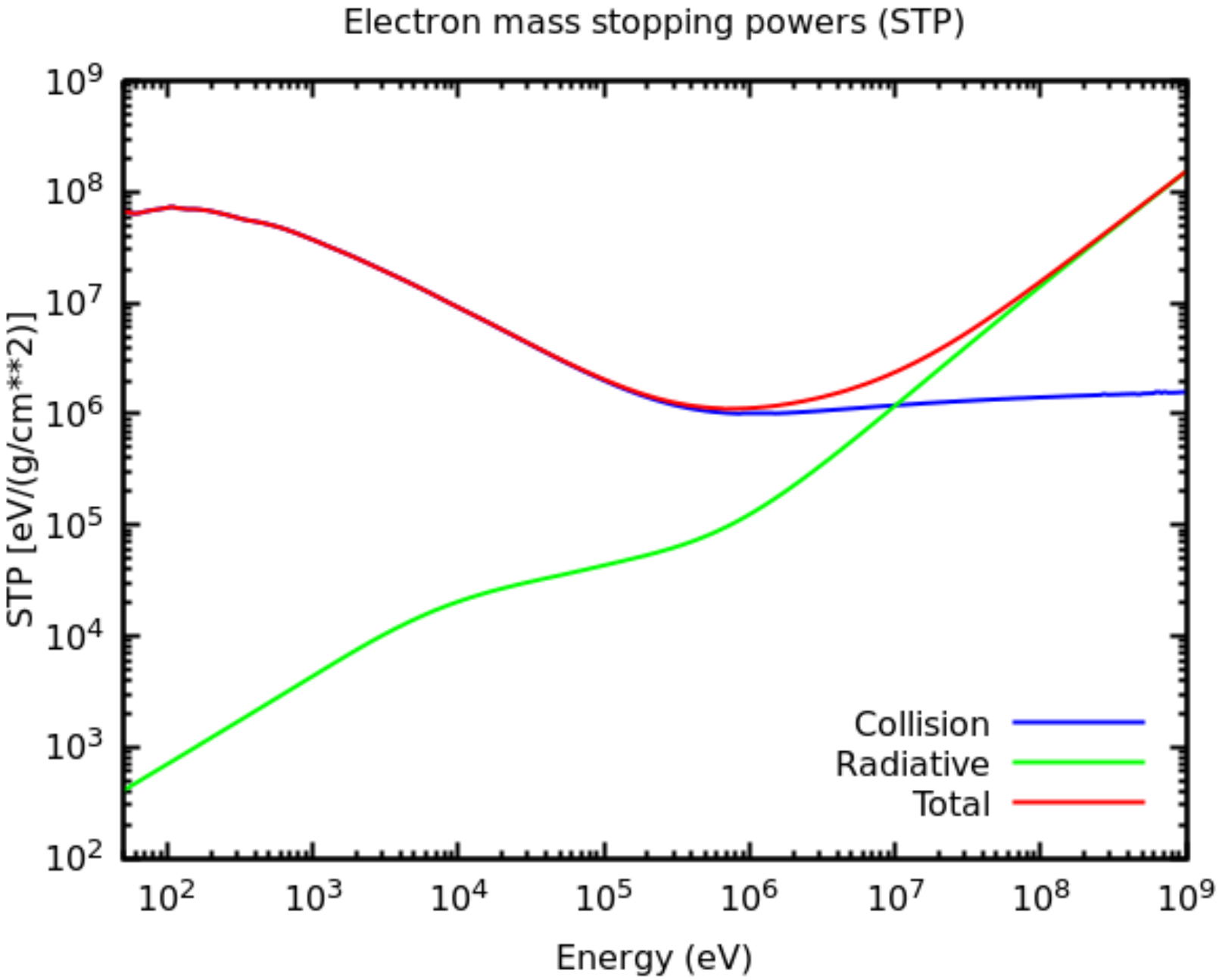


Figure 5.5. Differential cross-sections for elastic scattering of electrons by krypton atoms. Symbols represent experimental data from the quoted references. The solid curves represent DCSs calculated from the F–DF–FM potential. Dashed curves are results from calculations with the F–DF–FM–LDA–A optical model potential, with the default values of the potential parameters. Adapted from Salvat (2003).

2) Atomic inner-shell ionization by e^-/e^+ impact



Main energy loss mechanisms of electrons and positrons at low and moderate energies:



PHYSICAL REVIEW A **77**, 042701 (2008)

Calculations of inner-shell ionization by electron impact with the distorted-wave and plane-wave Born approximations

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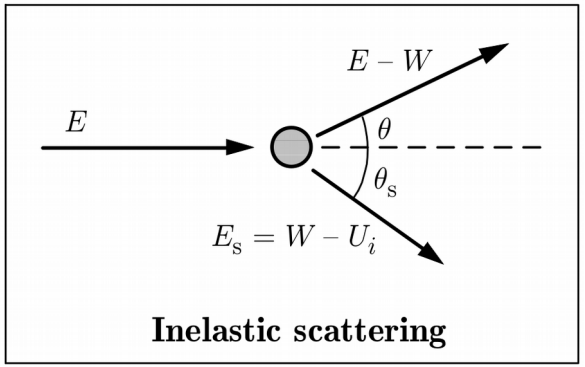
(Received 24 October 2007; published 1 April 2008)



- Historically: ~simple models (classical, non-relativistic, etc)
- PENELOPE: e^- spectroscopies (AES,EELS), microanalysis (EPMA), etc.
- Fairly detailed models needed: strict control on the underlying physics.
- Ionization cross sections calculated from first principles, relativistic (Dirac) DWBA (DHFS).
- Main idea: $T_{ba} = \langle \psi^{(-)}_{\mathbf{k}' m_{S'}}(0)\, \psi^{(-)}_{\mathbf{k}_b m_{Sb}}(1) | \mathcal{H}_{\rm int}(0,1) | \psi^{(+)}_{\mathbf{k} m_S}(0)\, \psi_{n_a \kappa_a m_a}(1) \rangle$
- Free states: plane waves distorted by atomic potential (nuc + ele self cons).
- Remaining perturbation (incident-outgoing electron inter) is small.
- Databases suited for simulation (adapted ene grids for accurate log-log interpolation). Usage of splines reduces database size.

PHYSICAL REVIEW A **77**, 042701 (2008)

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Primary energies above ~30 U_i → PWBA

Few data at the onset

Good point to remember yesterday's comment on typical order of magnitude for nuclear reactions

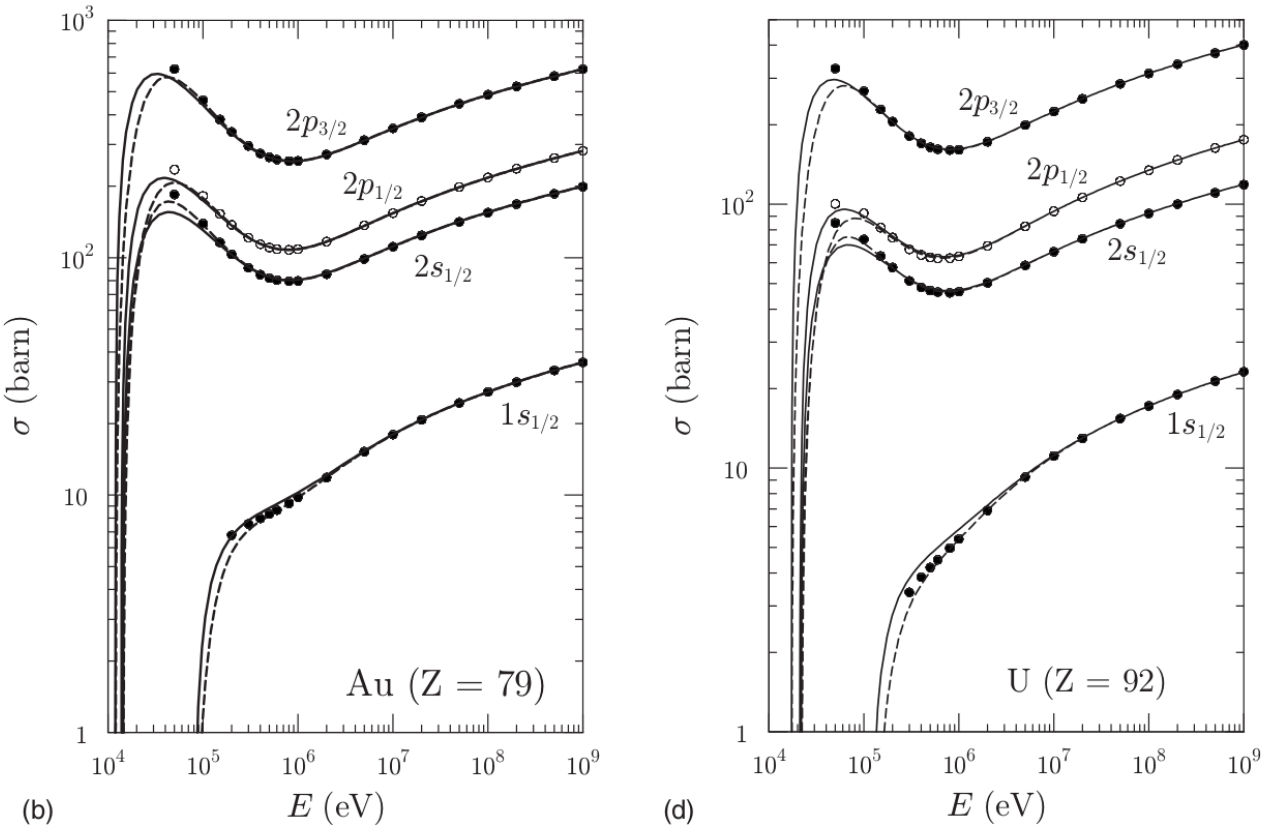

FIG. 4. Calculated total electron-impact ionization cross sections for the K shell and the L subshells of the indicated elements obtained from the present PWBA Eq. (77) (dashed lines) and from the corrected PWBA Eq. (99) (solid lines). Circles represent PWBA results from Scofield [12].

Ionization by e^-/e^+ impact

Cross Sections for Inner-Shell Ionization by Electron Impact

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(Received 7 November 2013; accepted 7 November 2013; published online 16 January 2014)

101 pages, theory and measurements.

Comparison theory/exp

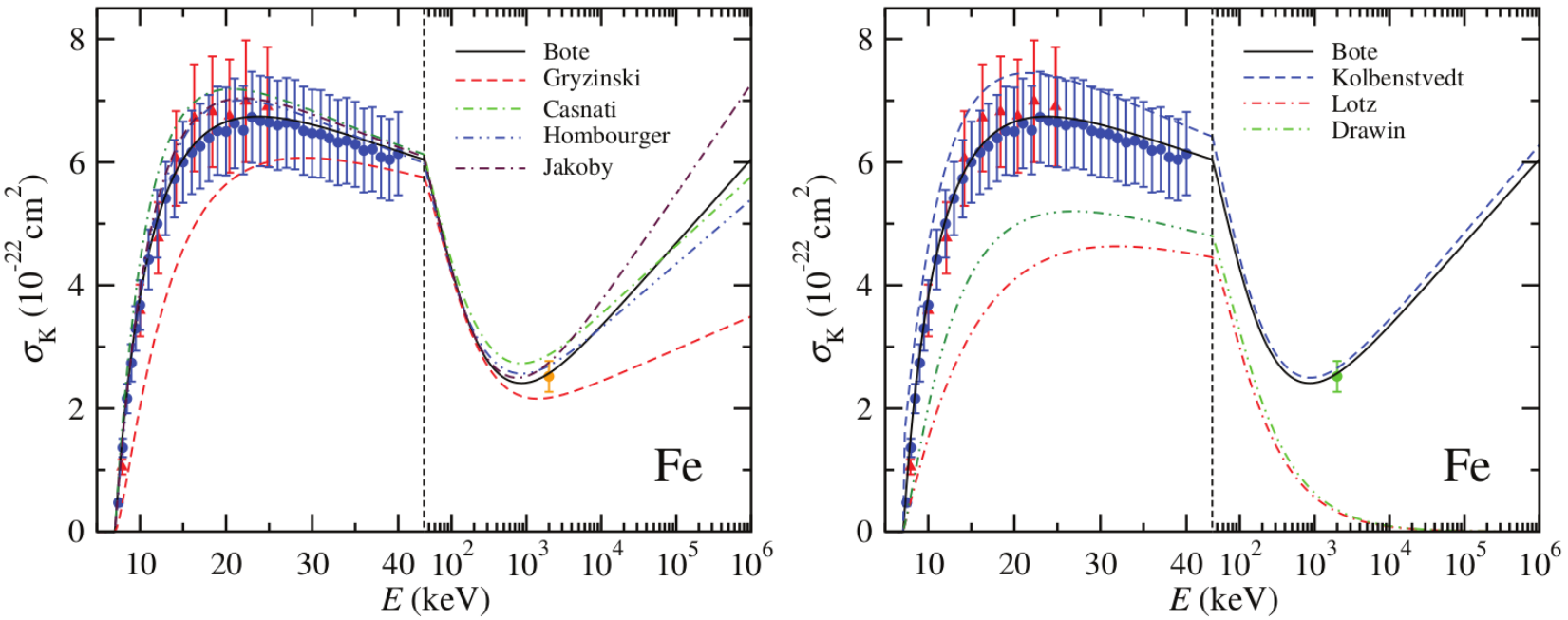


FIG. 7. (Color online) Absolute cross sections for ionization of the K shells of N, Si, Fe, Y, Ag, and Au *vs.* incident electron energy. The curves are the results of the DWBA calculations (solid lines) and of the analytical formulae indicated in the legends. The symbols represent experimental measurements that are identified in Sec. 6. The error bars are estimates of the one-standard-deviation uncertainties of the measured cross sections provided by the authors. Note the logarithmic scale in the high-energy parts of the horizontal axes.

Lack of experimental data at the higher energies
At lower energies: X. Llovet's measurements

Gryzinski, Casnati, Hombourger, Jakoby: empirical formulas

Low energy measurements (blue): EPMA on thin films

Main source of uncertainty: film thickness measurement

Onset correctly described by DWBA

N shells in PENELOPE

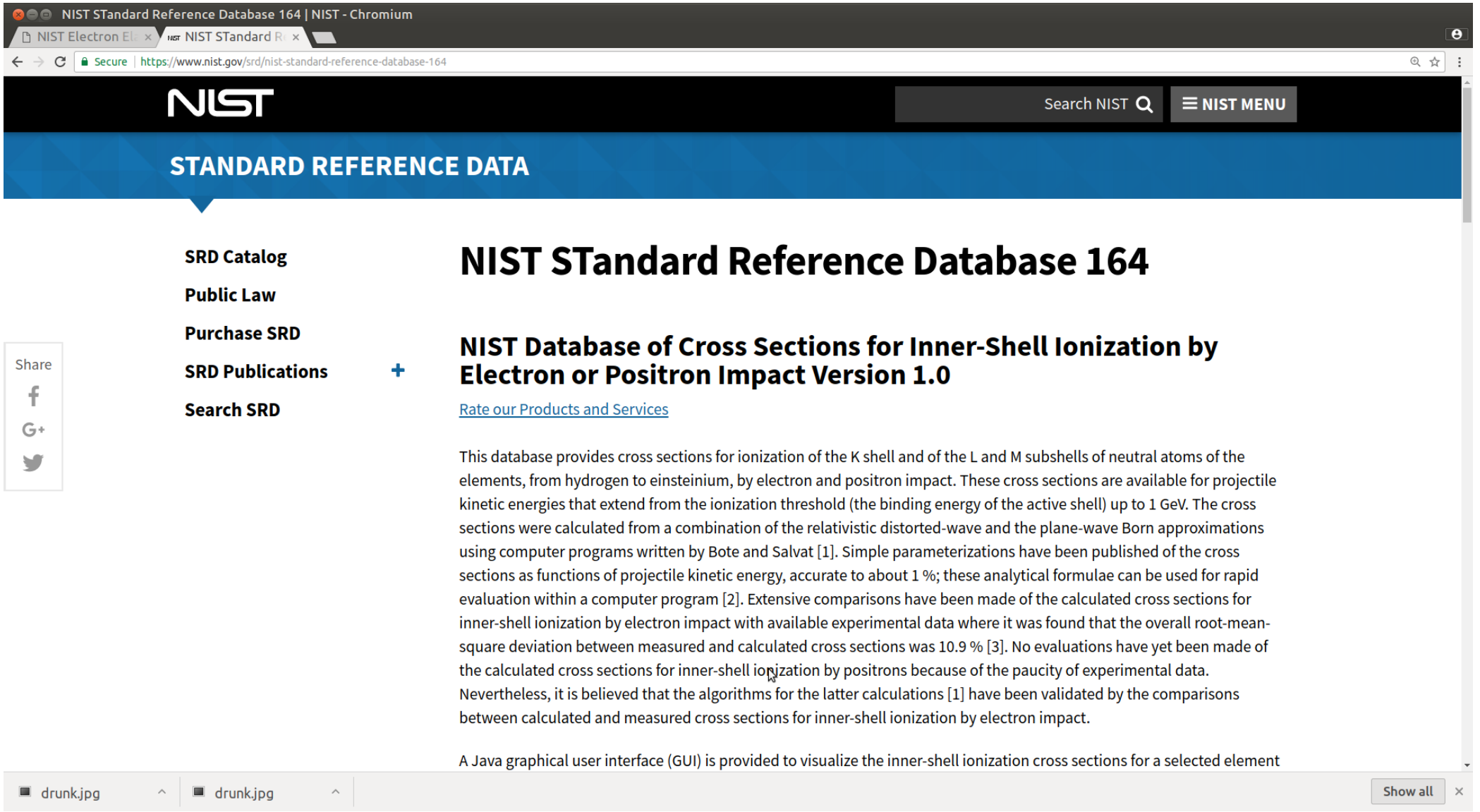
In MC codes with detailed model for ionization losses (usually for electron spectroscopies): K,L,M shells

In PENELOPE: K,L,M, **and N**

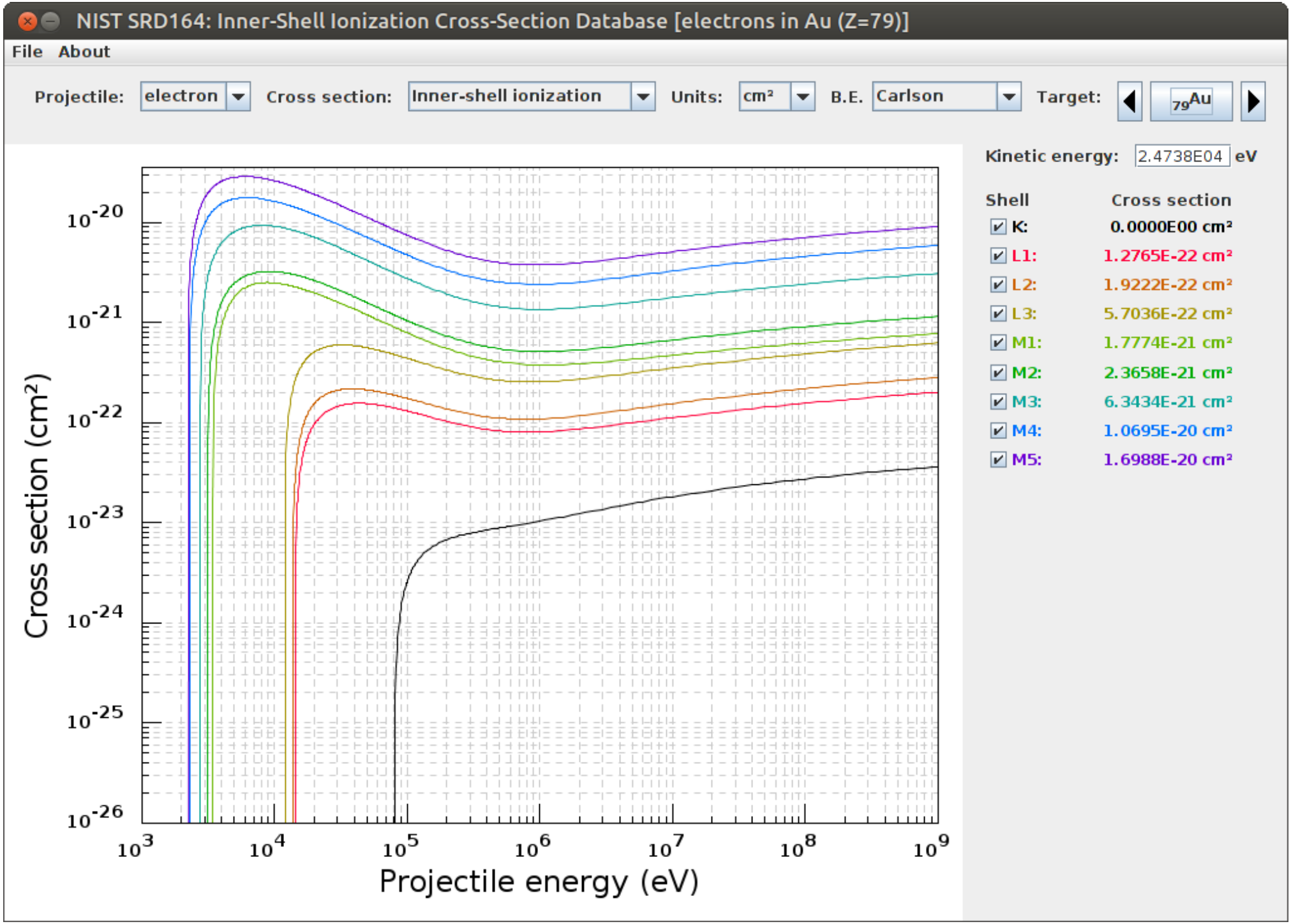
All calculated with same scheme

There are few measurements for N shell, e.g. Xe and heavy noble gases

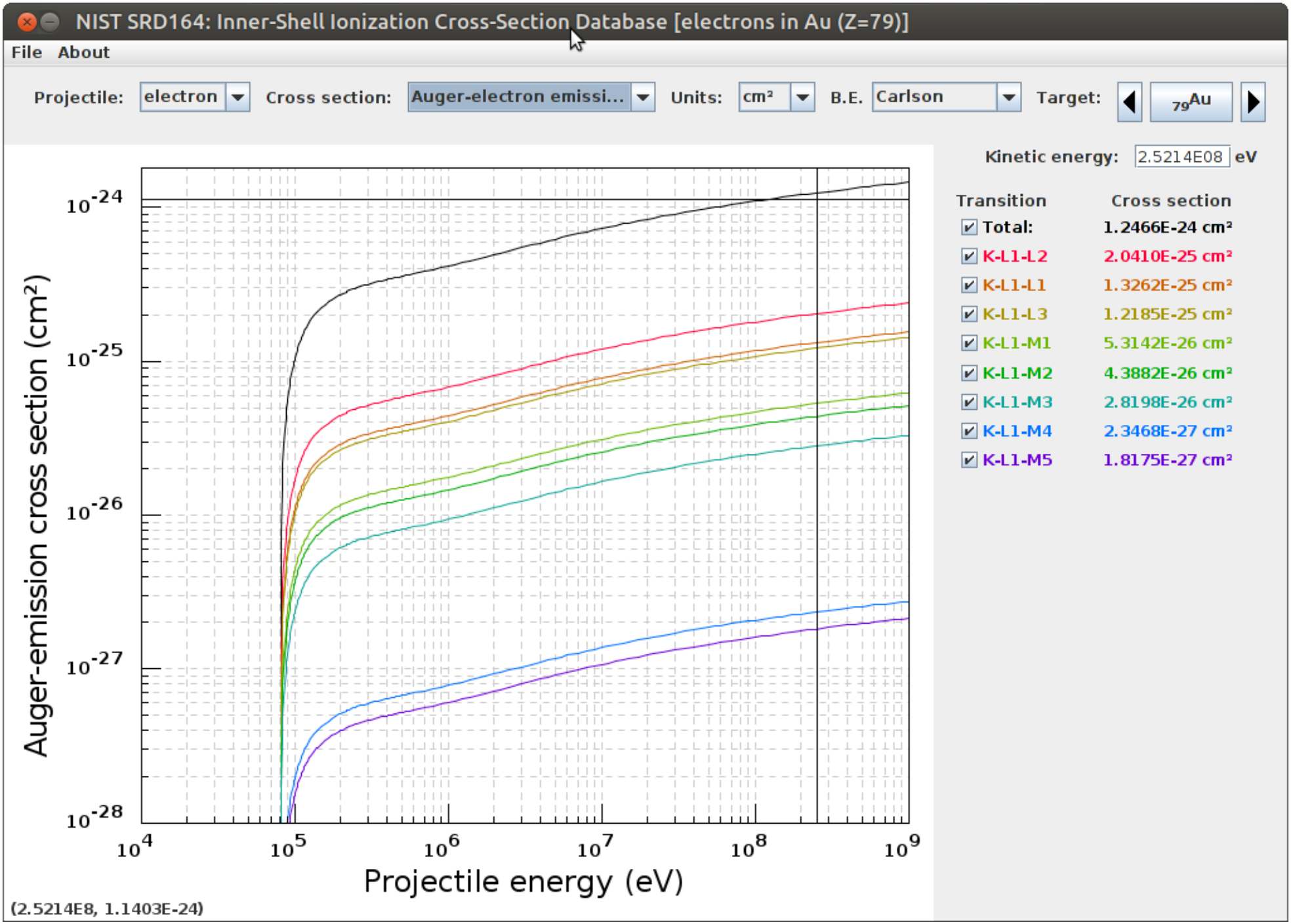
NIST SRD164 (2015)
K,L,M database + GUI



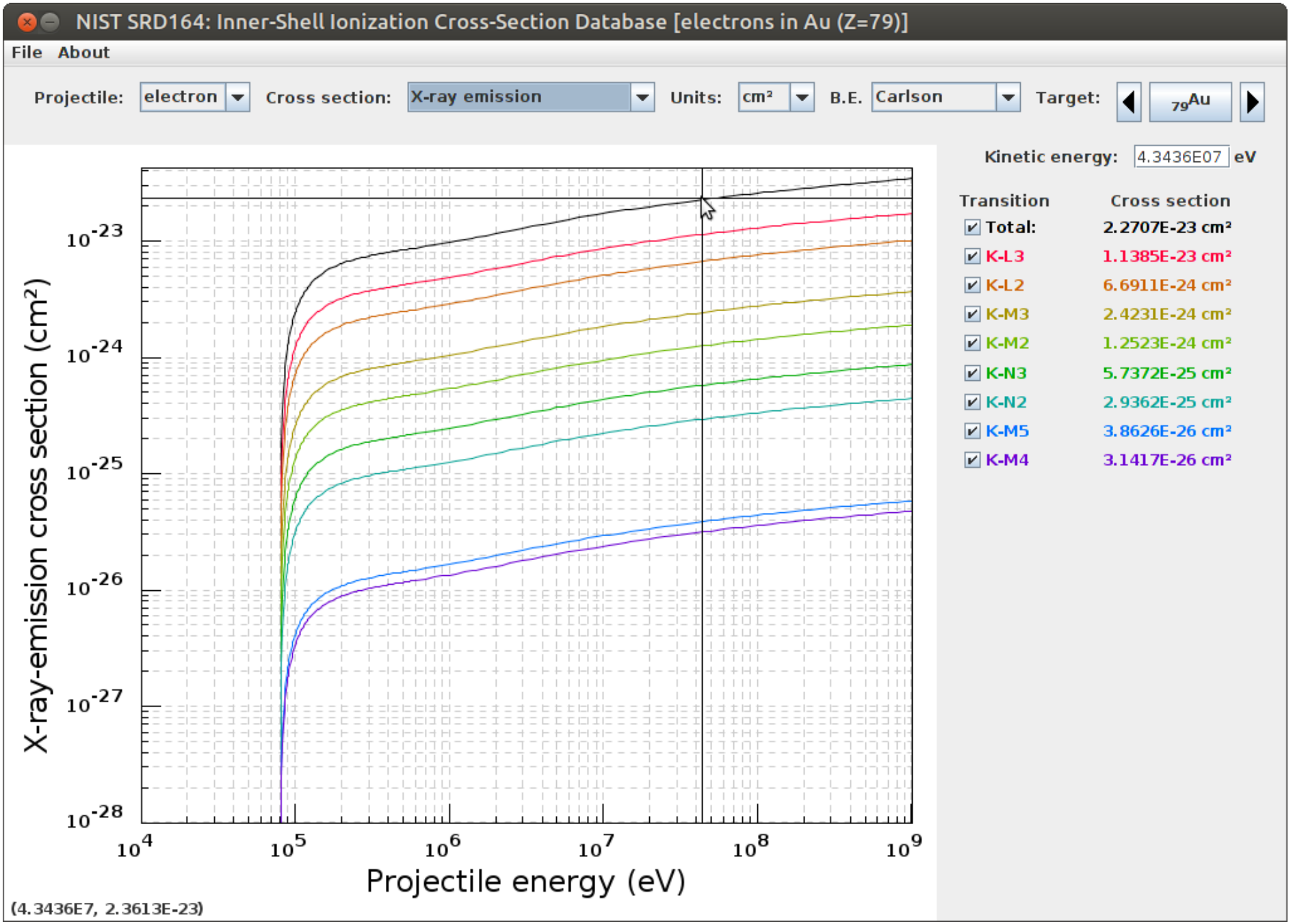
Inner-shell ionization cross section



Auger-electron emission cross section



X-ray emission cross section



Comparison electron/positron

Positron: lower ionization xs
(repelled by nucleus, arrives with less energy than electron would, not as effective at ionizing)
(electron on the other hand is attracted by the nucleus → more effective at ionizing)

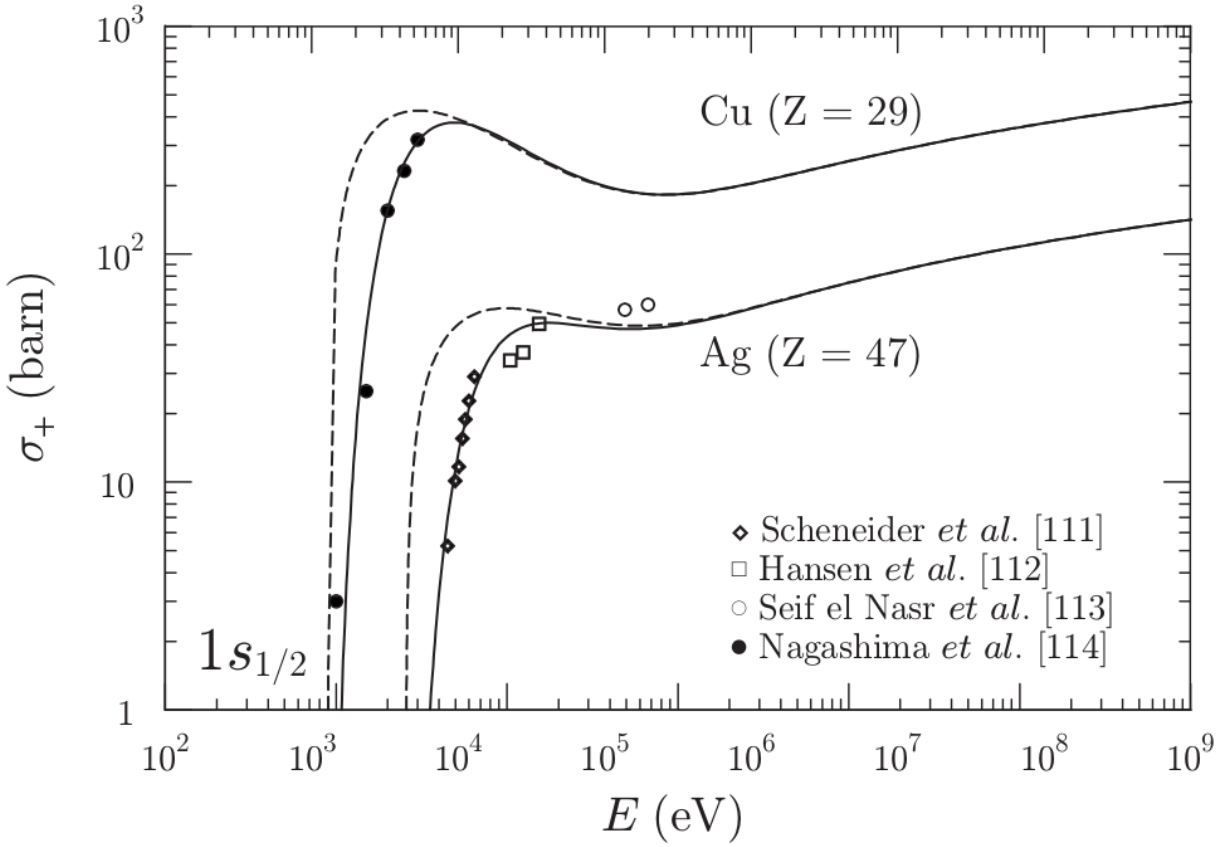
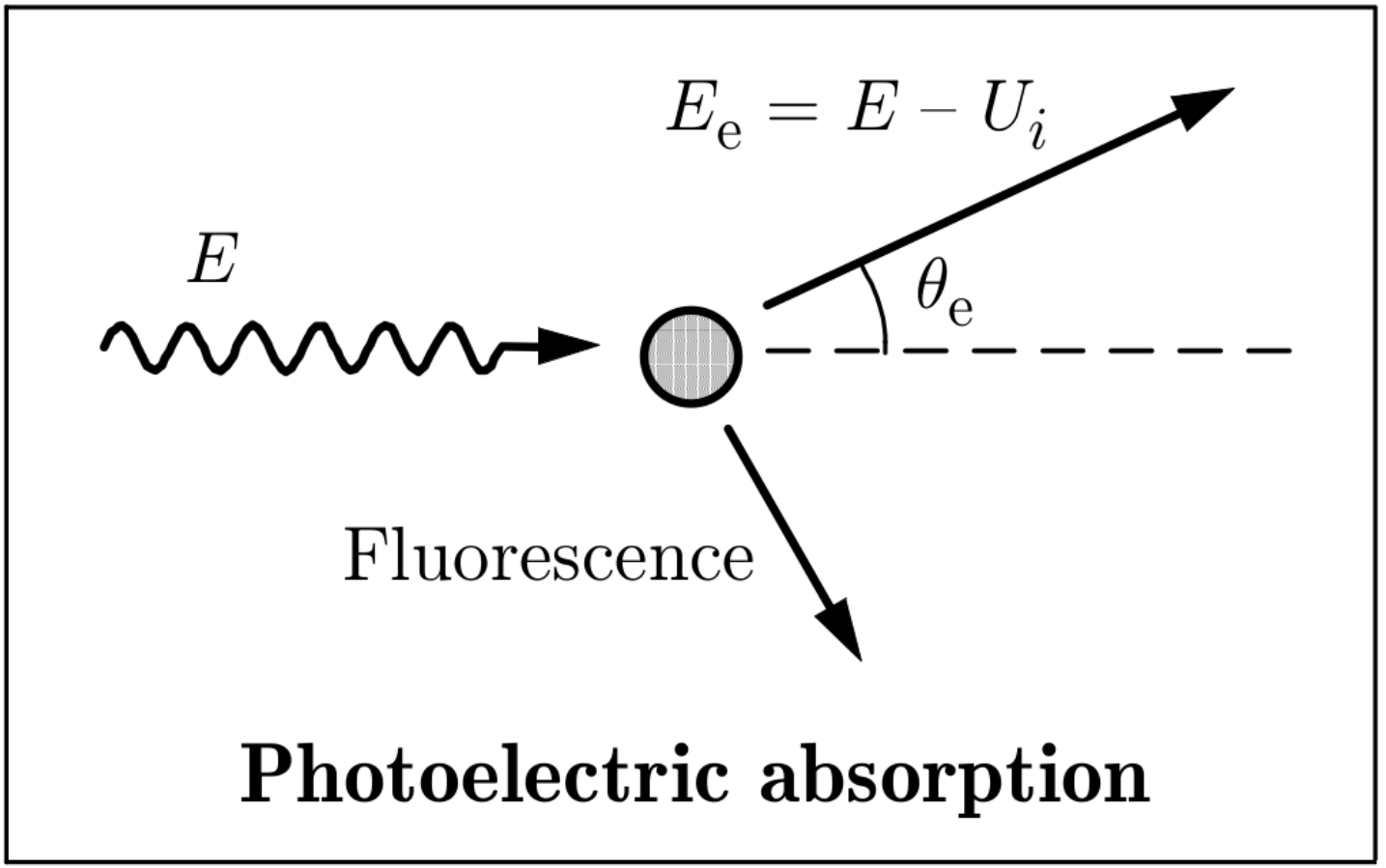


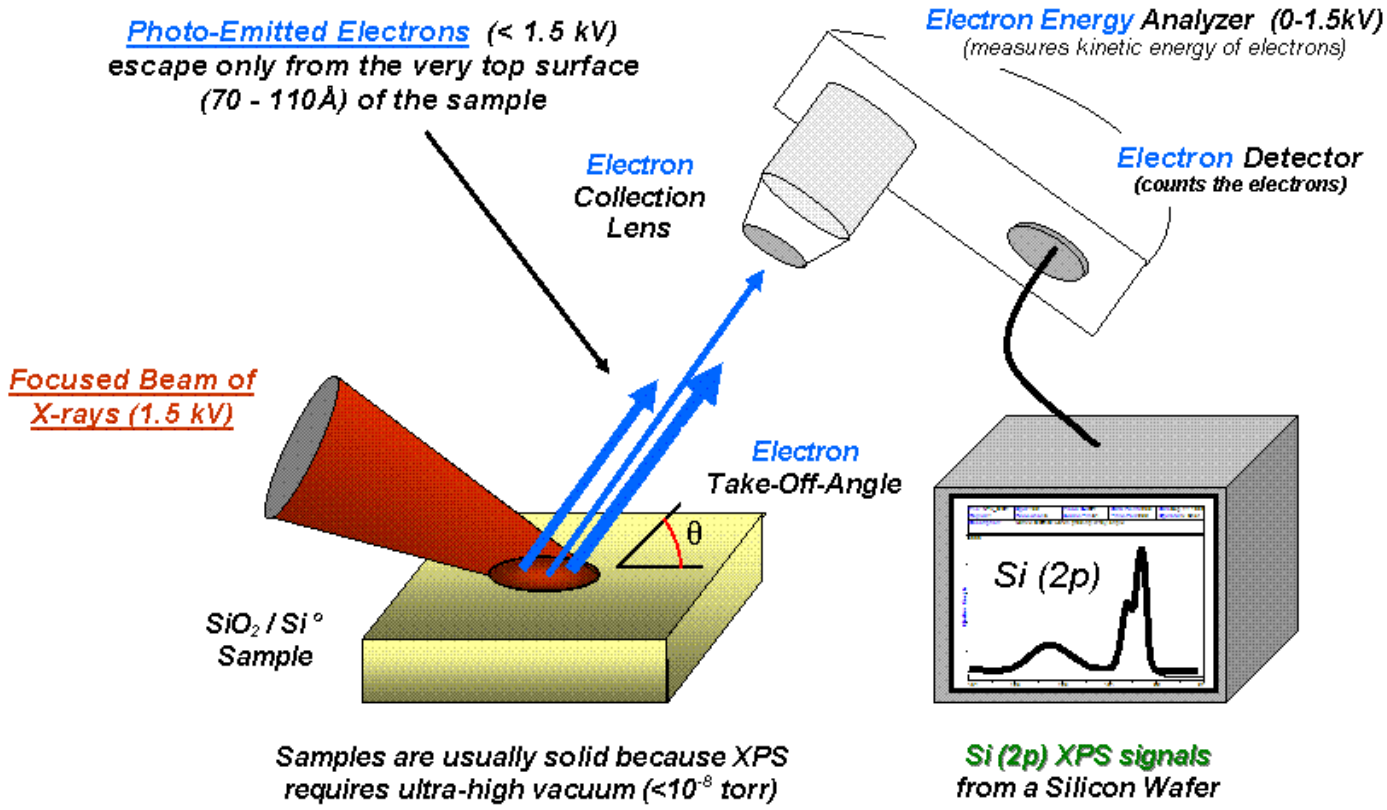
FIG. 8. Total cross sections for ionization of the K shell of the elements Cu and Ag by impact of positrons (solid curves) and electrons (dashed). Symbols represent experimental data for positrons [111–114].

3) Photoabsorption



Photoabsorption xs

- Surface spectroscopies (XPS) care about this

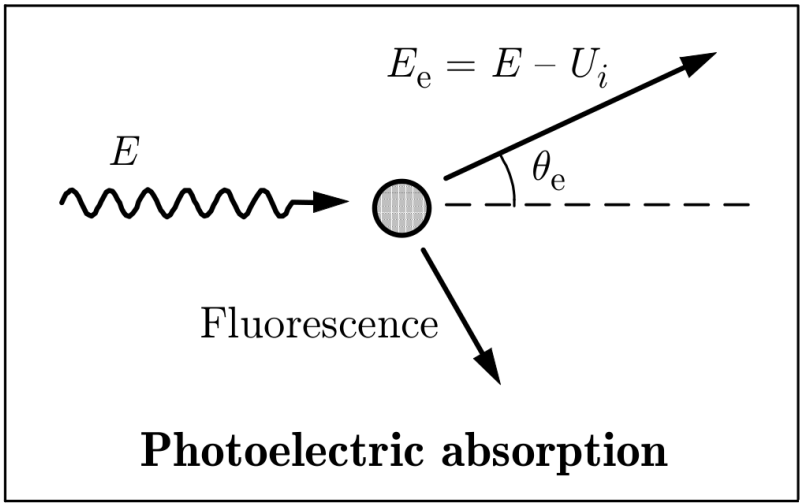


Source: wiki

- Peaks contain info about sample composition, chemical environment, etc.
- One needs reasonably detailed model.

Photoabsorption xs

- Typically: Evaluated Photon Data Library,
  compiled by Scofield & Hubbell (1997)
- Clients: surface spectroscopies (XPS), photon therapy
- A la PENELOPE: rigorous first-principles calculation.
- Atomic structure described by
  Dirac-Hartree-Fock-Slater self-consistent method
- Photon treated first order perturbation theory
  (photon PW, target e- bound → DW for ejected electron).
- In PENELOPE (and most MC): ionization only.



Radiation Physics and Chemistry 121 (2016) 122–140

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

journal homepage: www.elsevier.com/locate/radphyschem

Theory and calculation of the atomic photoeffect

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- Ionization AND excitation cross sections

  (e- promoted to unoccupied BOUND **orbital**).
- Angular distribution of photoelectrons: calculated directly, instead of using typical (in Monte Carlo) Sauter distribution (PWBA).

Photoabsorption (ioniztion AND excitation)

Below ionization thresholds there is contribution from excitation: e^- promoted to unoccupied BOUND orbital.

Excitation region is made continuous by Lorentzian convolution with empirical atomic level width (vacancy life time)

Is seen in K, L, and most visibly M shells

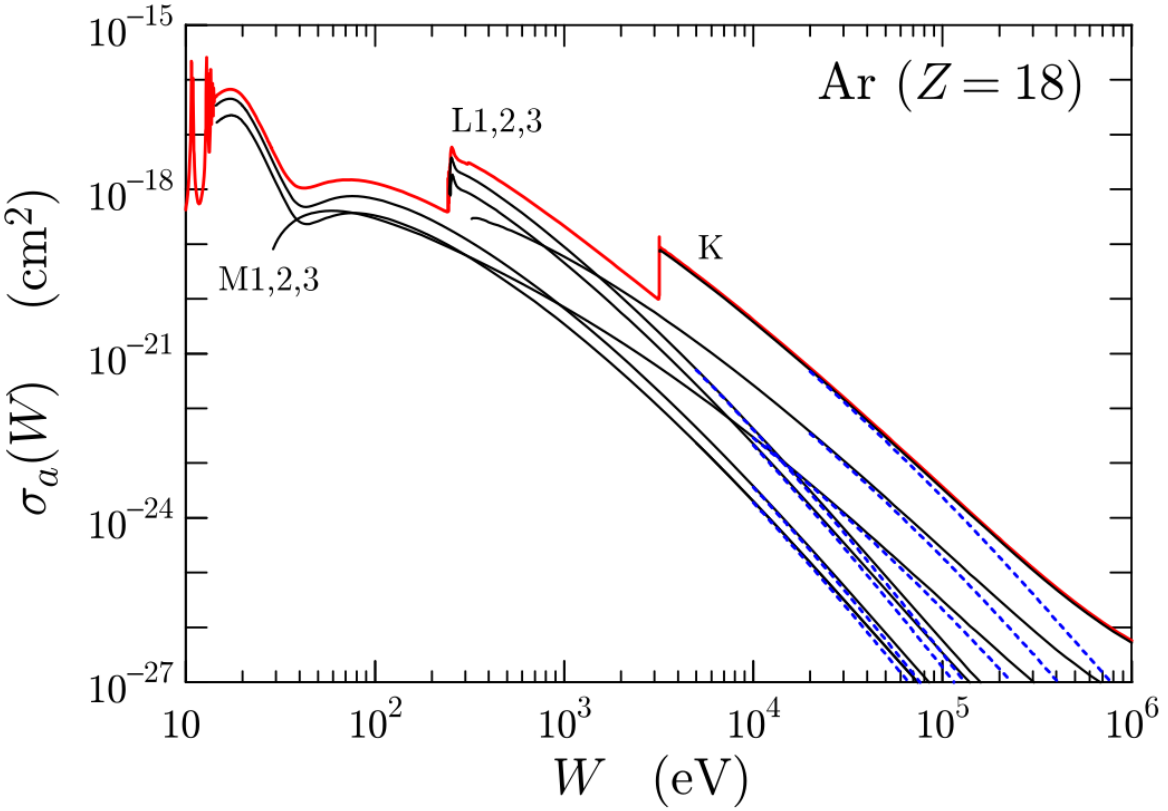


Fig. 4. Cross sections for photoabsorption (excitation and ionization) in the subshells of argon atoms as functions of the photon energy W (thin solid curves), calculated by PHOTACS-PP using experimental level widths. The thick solid curve (red online) represents the total atomic cross section. Dashed curves (blue online) are cross sections obtained from the dipole approximation. (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this paper.)

Photoelectron angular distribution

- Typically only K-shell hydrogen-like model of Sauter (PWBA).

PHOTACS can calculate for any shell

Here we show K shell for comparison

Even in favorable K-shell case, Sauter departs from DWBA at large angles (!)

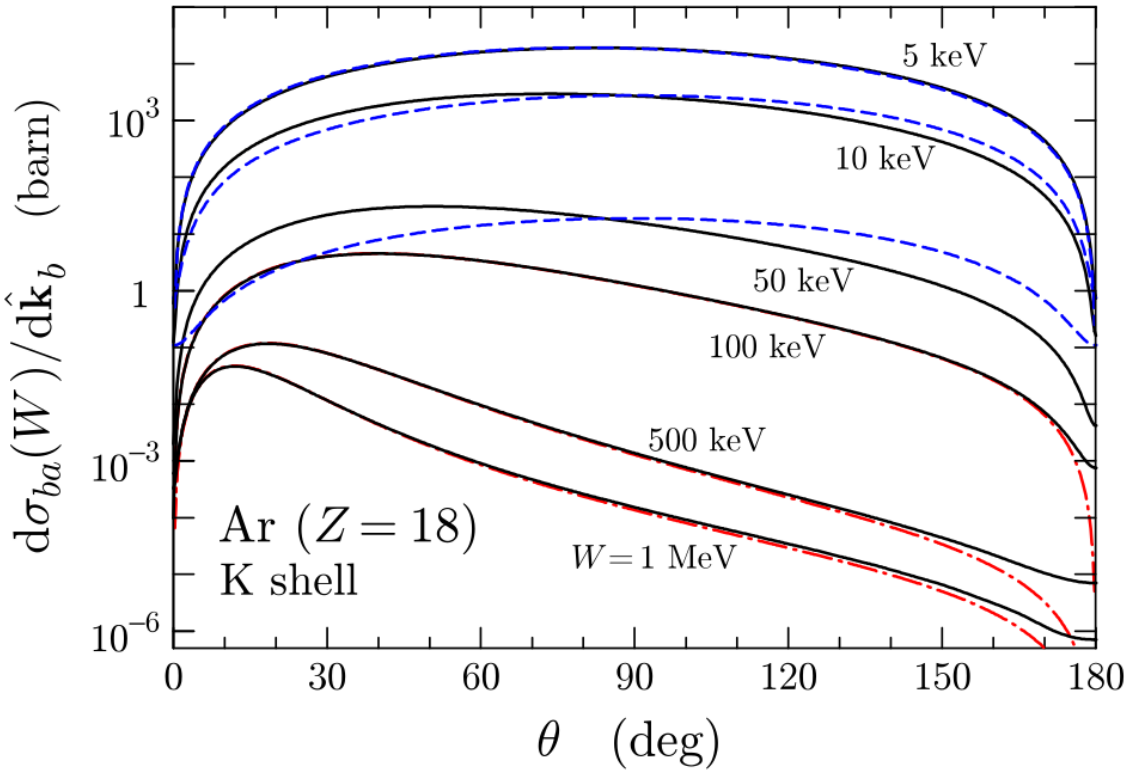


Fig. 5. Differential cross sections for ionization of the K shell of argon atoms by unpolarized photons of the indicated energies. Solid curves represent partial-wave numerical results. Dashed curves (blue online) are results from the dipole approximation. Dot-dashed curves (red online) correspond to the Sauter distribution, Eq. (65), multiplied by the numerical total cross section calculated from Eq. (16). (For interpretation of the references to colour in this figure caption, the reader is referred to the web version of this paper.)

Absorption of polarized photons

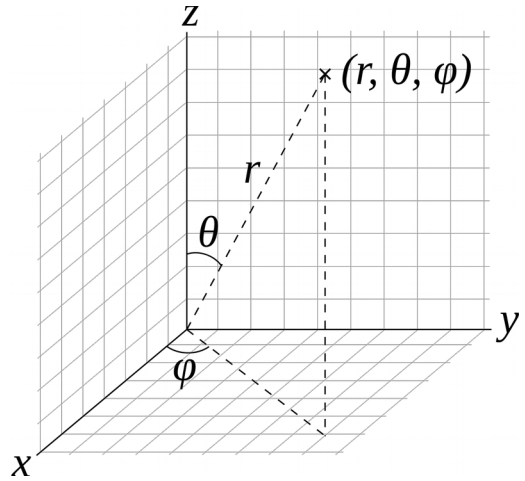
50-keV polarized photons
on K shell of Ar

Polarization ~ direction of oscillation of electric field

→ Photoelectrons emitted preferentially in polarization direction.

Top: photon polarized along the y axis
Th = 90, Phi = 90, 270

Bottom: polarization on
Th = 90, Phi = 45, 225



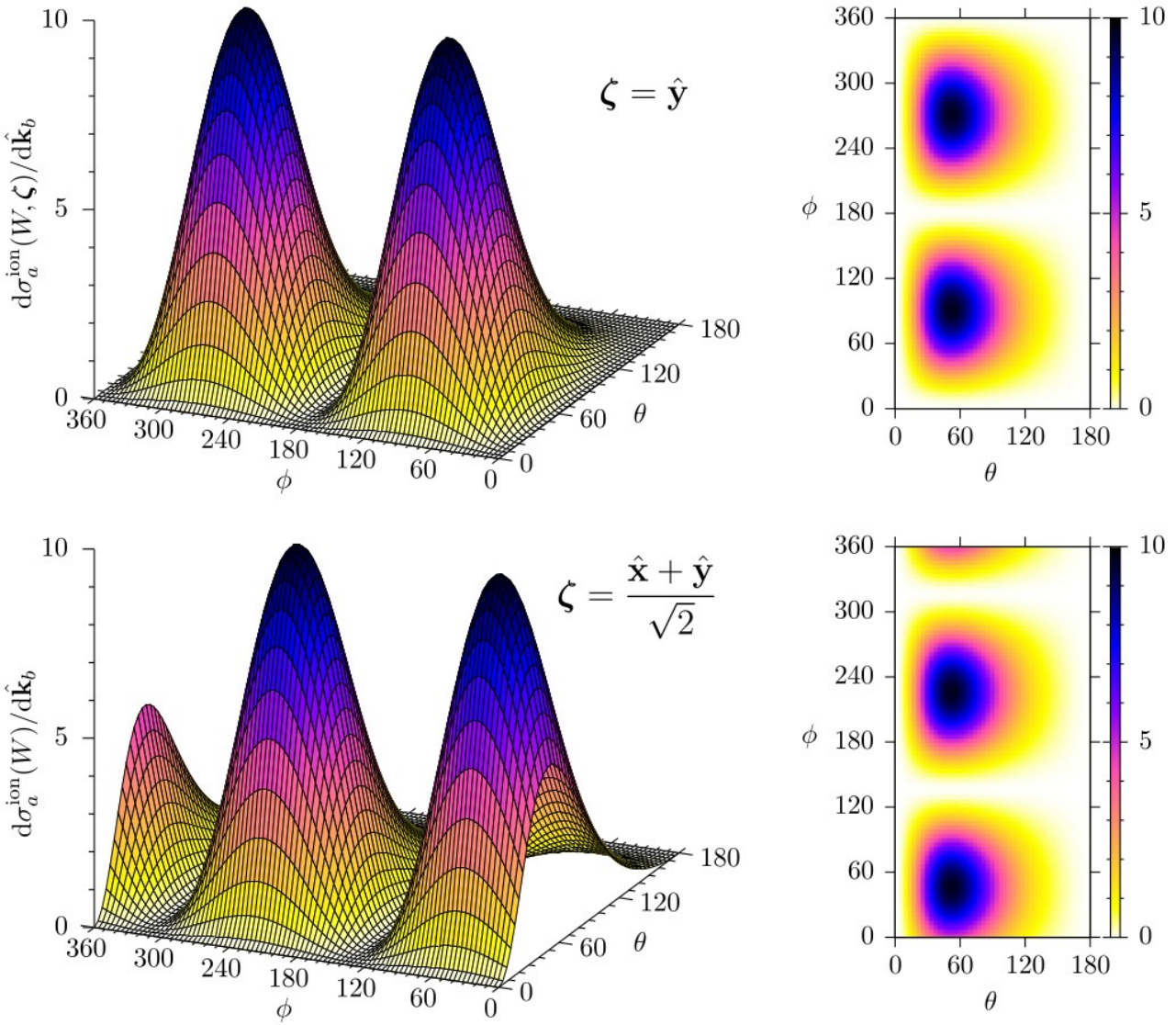


Fig. 6. DCSs for ionization of the K shell of Ar atoms by absorption of 50 keV photons, in barn (=10^{-24} cm^2), as functions of the polar angle θ and the azimuthal angle ϕ of the direction of the emitted photoelectron, both in degrees. The plots correspond to photons linearly polarized along the x-axis [$\mathbf{P} = (0, 0, 1)$, top], along the y-axis [$\mathbf{P} = (0, 0, -1)$, middle], and along the direction $\hat{\boldsymbol{\xi}} = (\hat{\mathbf{x}} + \hat{\mathbf{y}})/\sqrt{2}$, at 45° from the x-axis [$\mathbf{P} = (1, 0, 0)$, bottom].

4) PENH

PENH

- Extend PENELOPE transport scheme so as to include p transport
- Class II: condensed below ene/ang cutoff, detailed above
- Electronic stopping (including inner shell ionizations)
- Potential scattering (including nuclear recoils)
- Developed for p-induced x-ray emission (PIXE)

Nuclear Instruments and Methods in Physics Research B 316 (2013) 144–159

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Nuclear Instruments and Methods in Physics Research B

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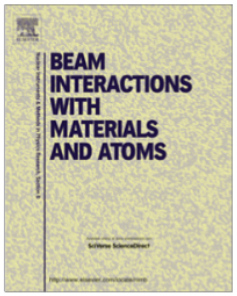

A generic algorithm for Monte Carlo simulation of proton transport

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PENH: potential scattering

DWBA not feasible for p on full atomic potential (considering electron screening)
Implies integrating radial equations numerically.

Eikonal approximation with spin-relativistic corrections.

Cross sections for p do not exhibit as much structure as for electrons
(p have much shorter deBroglie wavelength → go back and show on plot)

Just for comparison: dashed PWBA (only at high)

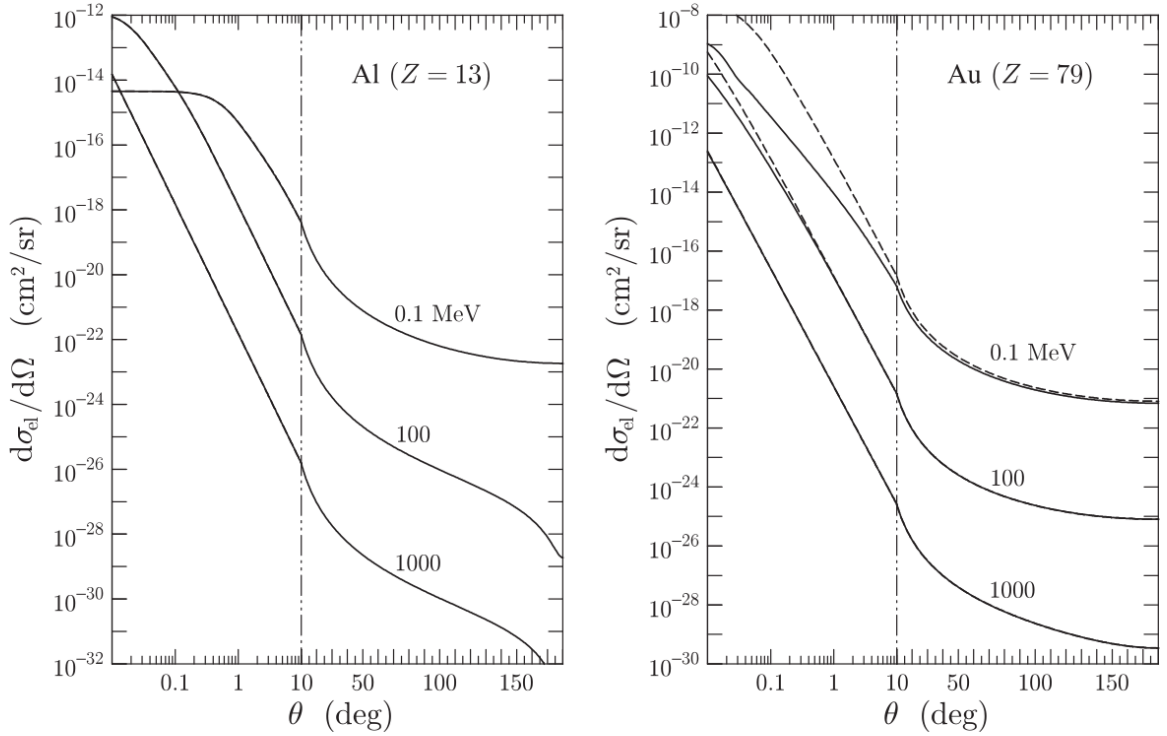


Fig. 1. DCS for elastic scattering of protons with the indicated kinetic energies by Al and Au atoms, calculated with the eikonal approximation for the DHFS potential, Eq. (33). The dashed lines represent the DCS obtained from the Born approximation, Eq. (16), multiplied by the spin factor $1 - \beta^2 \sin^2(\theta/2)$. Note the change of scale on the horizontal axes.

Inner-shell ionization by proton impact

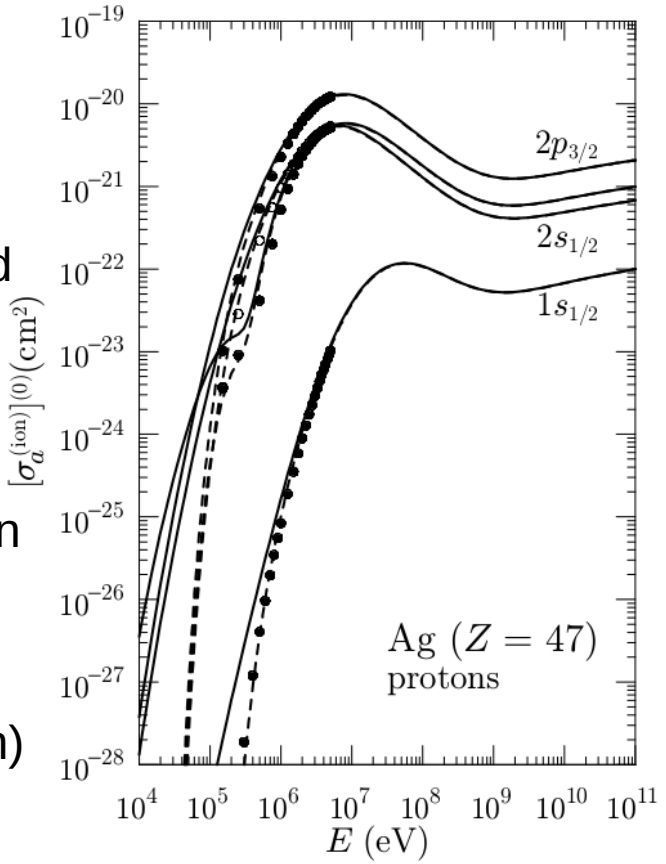
Similar numerical machinery
as for ele/posi impact

Based on PWBA+corrections
~DWBA

Ionization xs can be calculated
as easily for protons

Solid curves: PWBA
Dashed: PWBA+corrections
Symbols: equivalent calculation
by Chen&Crasemann

Standard in PIXE
(Proton induced x-ray emission)



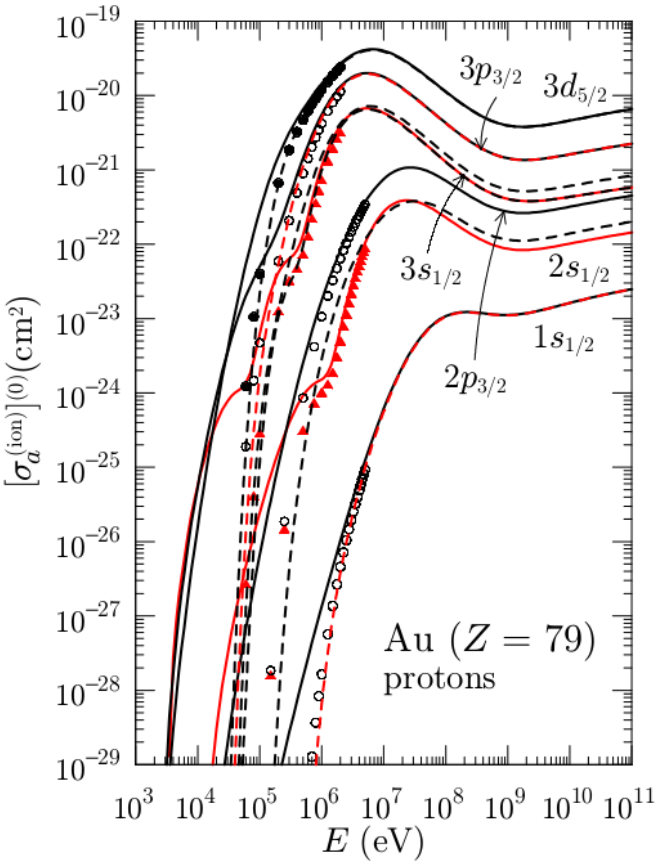


Figure 12.1: Total cross sections for ionization of the indicated (K, L and M) shells of titanium, germanium, silver and gold by impact of protons as functions of the kinetic energy of the projectile. Solid curves were calculated by using the unmodified PWBA, the dashed curves represent results from the PWBA with binding and Coulomb-deflection corrections, Eq. (12.14). Symbols are results from equivalent PWBA calculations by Chen and Crasemann (1985, 1989), which also include these low-energy corrections.

Example: transmission through thin films

Results of class II simulation of proton transport with PENELOPE

Relative shape comparison only
(measurements normalized to MC).

Proton physics are of the same quality as rest of PENELOPE transport model.

Expected good agreement is indeed found.

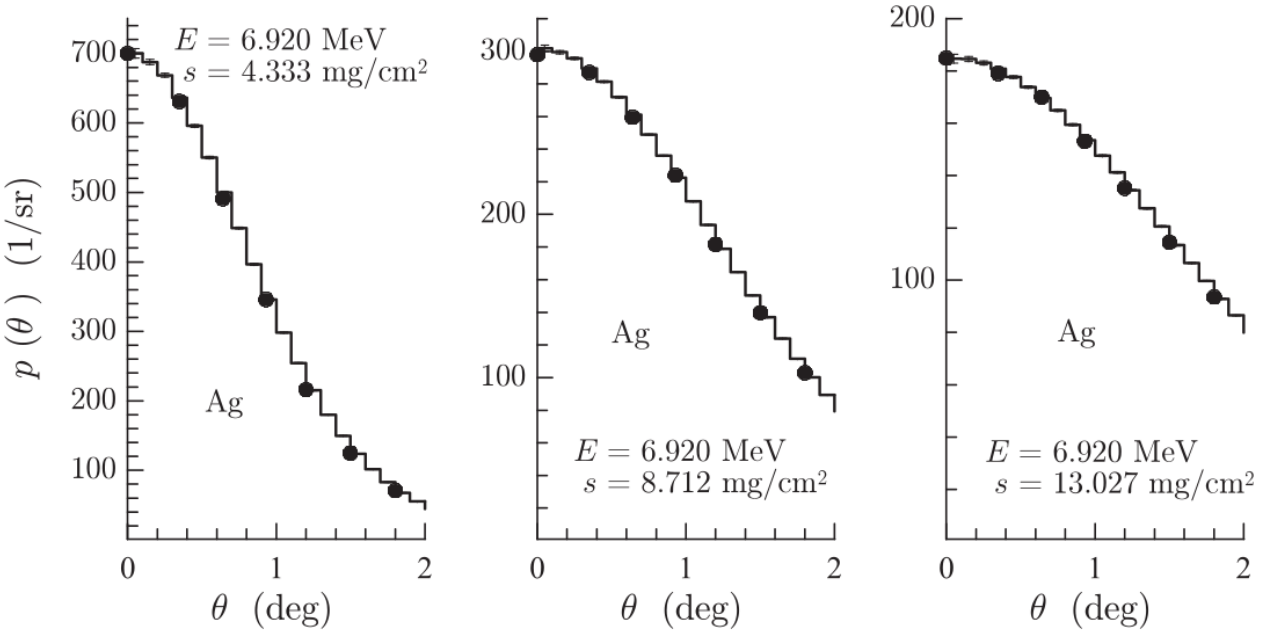


Fig. 3. Angular distributions of protons transmitted through thin Al and Ag foils. Solid circles represent relative measurements of Ishiwari et al. [51], normalized at $\theta = 0$. Solid histograms are results from simulations with the PENH subroutines, obtained with conservative values of the simulation parameters ($C_1 = C_2 = 0.0001$, W_{cc} = 2.5 keV). Error bars represent statistical uncertainties (3σ).

5) Radioactive sources

Not PENELOPE’s main aim
but friends from CIEMAT needed it

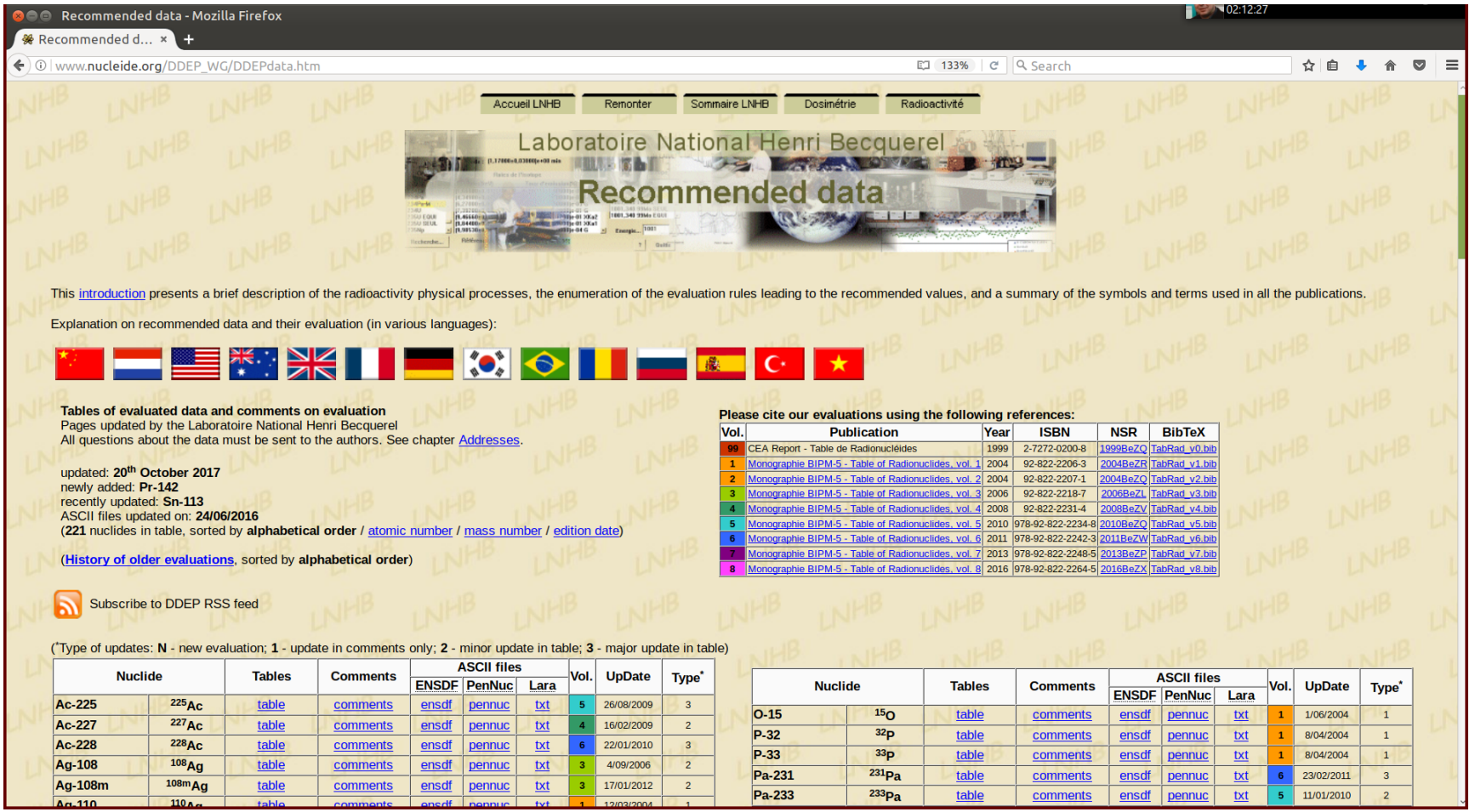
PENELOPE actually started after a MC course in CIEMAT 1987 to satisfy simulation needs of radiation metrology group

PENNUC

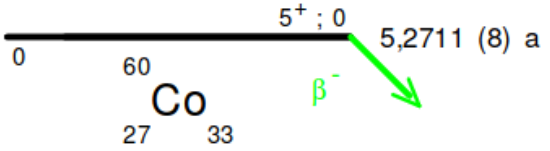
Adapted penmain.f (source subroutine samples radioactive decay)

NUCLEIDE: evaluated database

Given a radionuclide, simulate de-excitation cascades and emission times



PENNUC

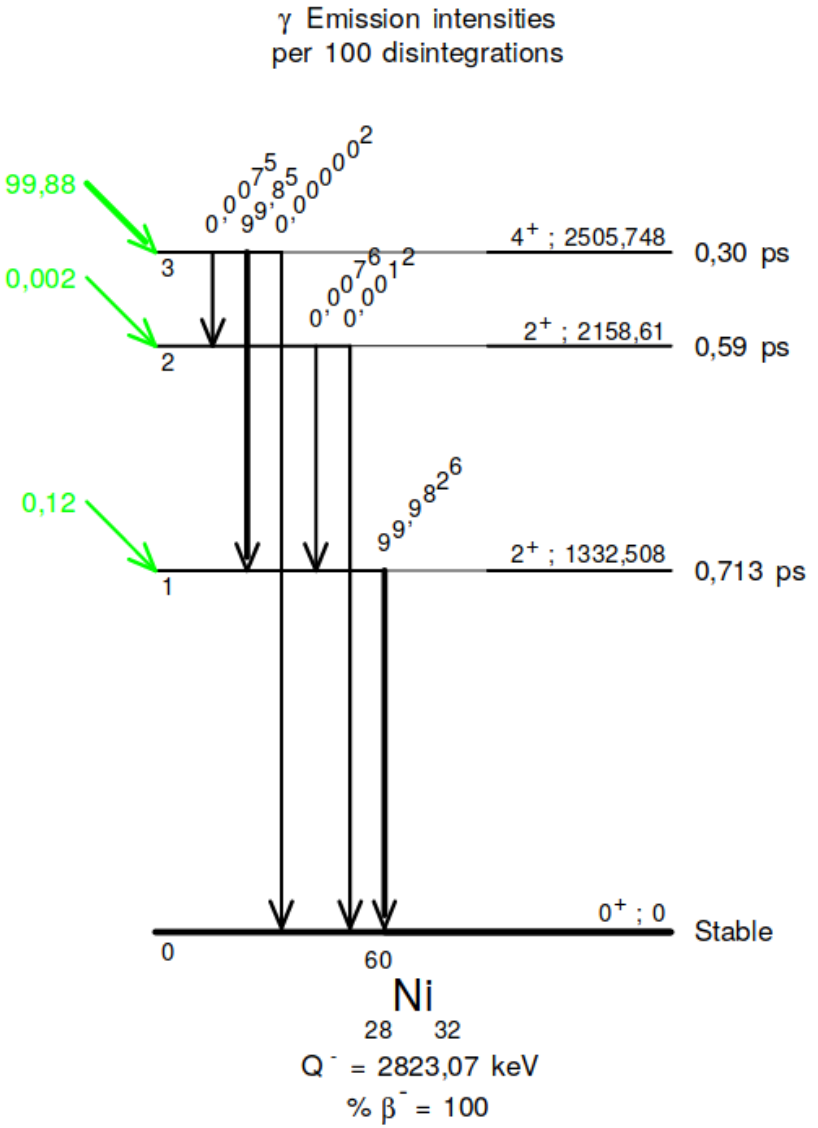


General problem: simulation of radioactive sources (beta+-, photons).

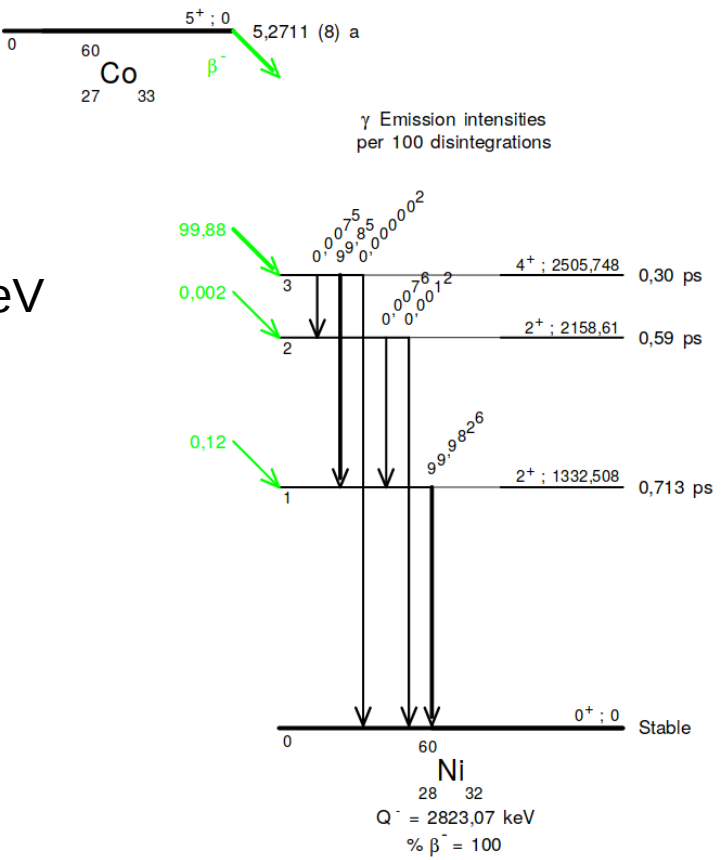
Given a radionuclide, decay scheme can be obtained in pennuc format from nucleide.org

a) Allows for ~easy evaluation of dose or energy spectrum deposited in detector given a radioactive source
(no need to program all decay scheme)

c) Detector efficiency: accounts for peak summing effects (e.g. one ^{60}Co)



Radiation detector efficiency



Example issue: ^{60}Co (1.33 and 1.17 MeV photons).
Coincidence-summing artifact
If time resolution of detector is not fine enough, hit 1.33+1.17 MeV
Reduction in 1.33 MeV and 1.17 MeV peaks
Apparent loss of efficiency
MC simulation with both photons → correct peak areas

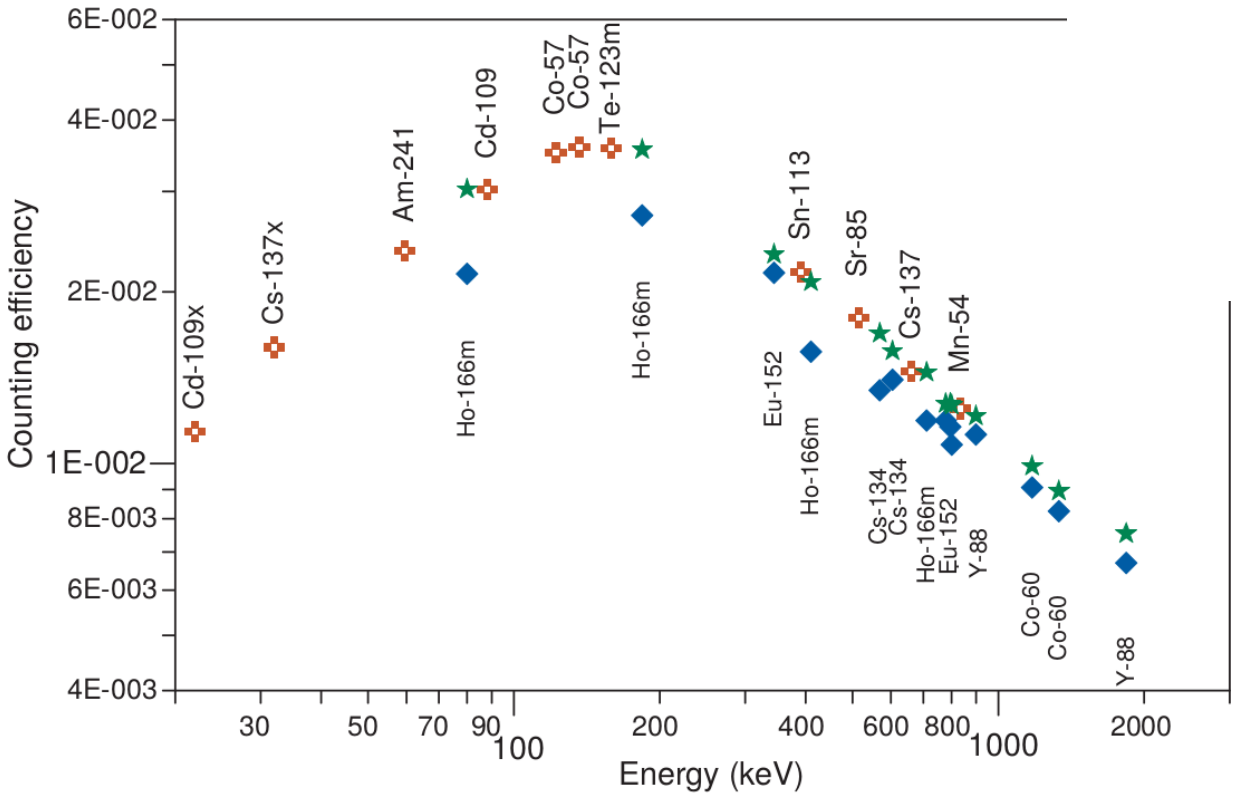


Fig. 1. Measured efficiency curve for System I (Marinelli beaker). Crosses correspond to γ-ray lines not affected by coincidence-summing and diamonds to the values obtained for γ lines with significant coincidence-summing effects. Efficiencies obtained in the simulation for the multi-γ emitters, corrected by coincidence-summing, are represented by stars. To improve the readability of the figure, several overlapping results have been omitted.

Radiation detector efficiency

Nuclear Instruments and Methods in Physics Research B 396 (2017) 43–49

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Nuclear Instruments and Methods in Physics Research B

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Simulation of decay processes and radiation transport times in radioactivity measurements

E. García-Toraño [a,*], V. Peyres [a], M.-M. Bé [b], C. Dulieu [b], M.-C. Lépy [b], F. Salvat [c]

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[b] CEA, LIST, Laboratoire National Henri Becquerel (LNE-LNHB), Bldg 602, PC111, 91191 Gif-sur-Yvette Cedex, France
[c] Facultat de Física (FQA and ICC), Universitat de Barcelona, Diagonal 647, 08028 Barcelona, Spain

6) Graphical tools

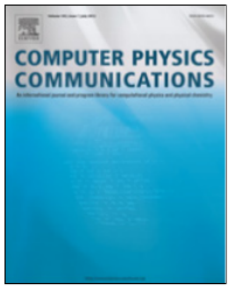
PENGEOM

Computer Physics Communications 199 (2016) 102–113

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc



PENGEOM—A general-purpose geometry package for Monte Carlo simulation of radiation transport in material systems defined by quadric surfaces☆

Julio Almansa [a], Francesc Salvat-Pujol [b], Gloria Díaz-Londoño [c], Artur Carnicer [d], Antonio M. Lallena [e], Francesc Salvat [d,*]

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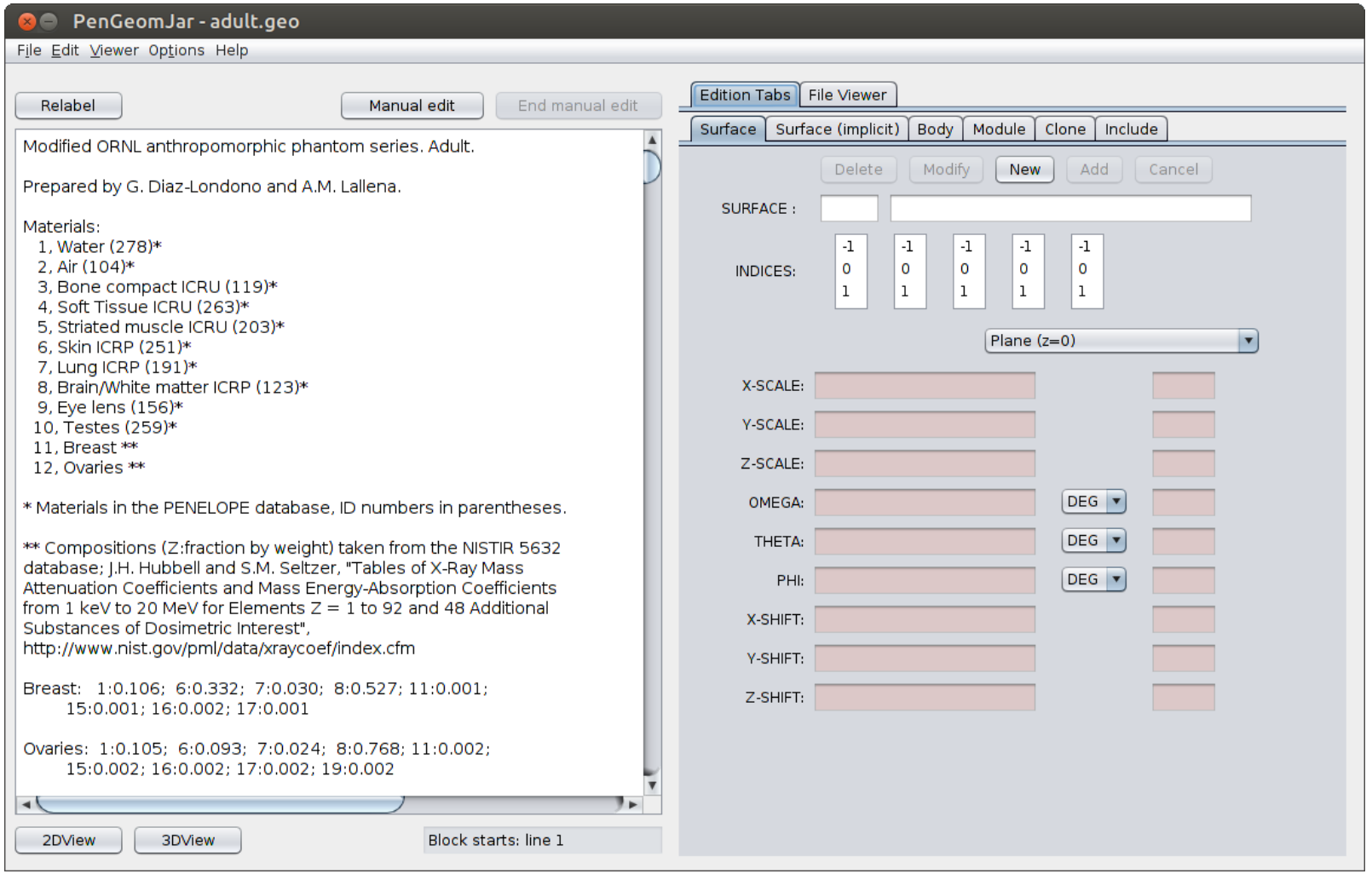
PenGeomJar

Windows, Linux, Mac

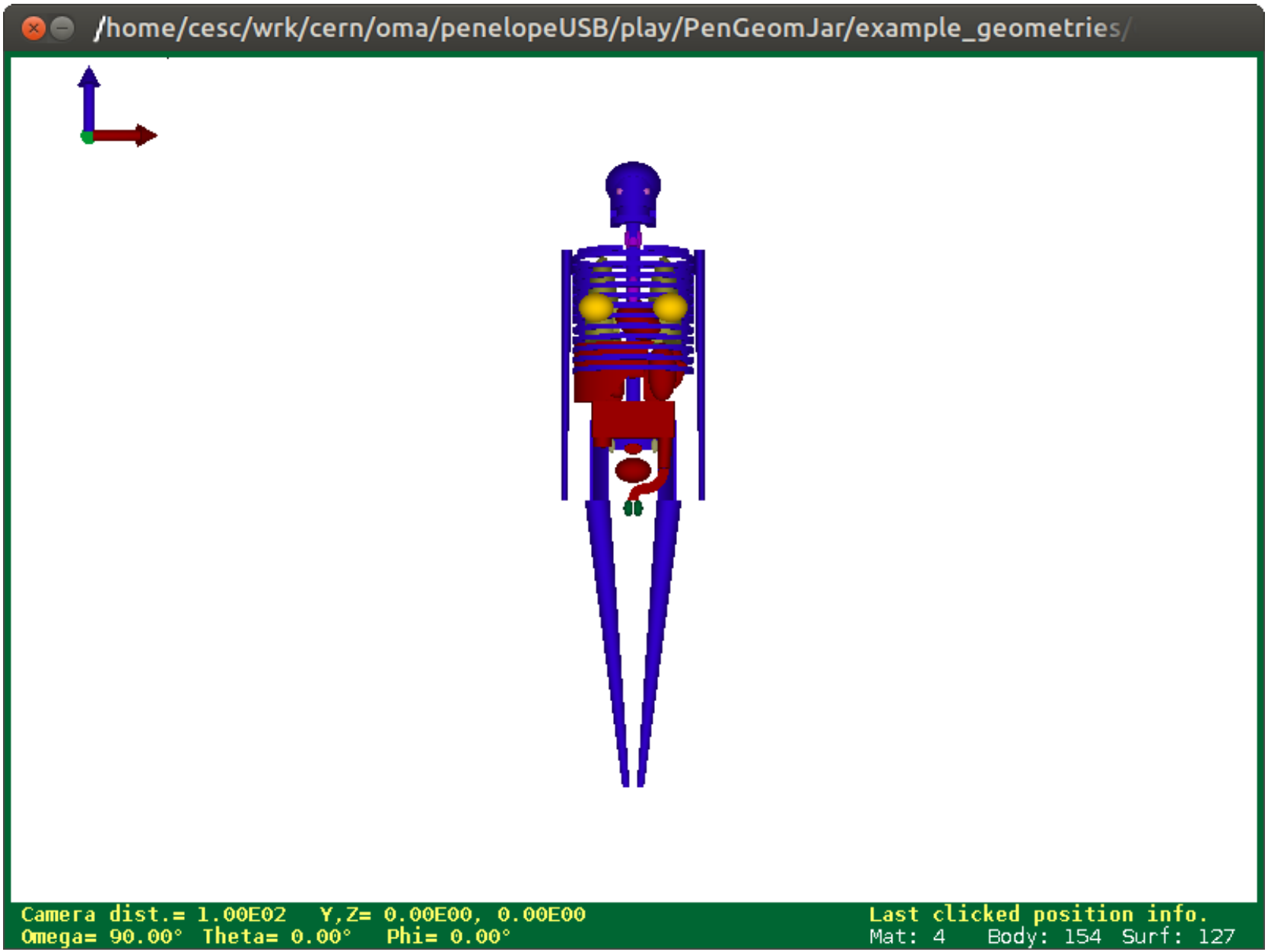
Like all PENELOPE programs, free.

Edit and visualize geometry input file

RAY TRACING WITH PENELOPE TRACKING! What you see is what PENELOPE sees



PenGeomJar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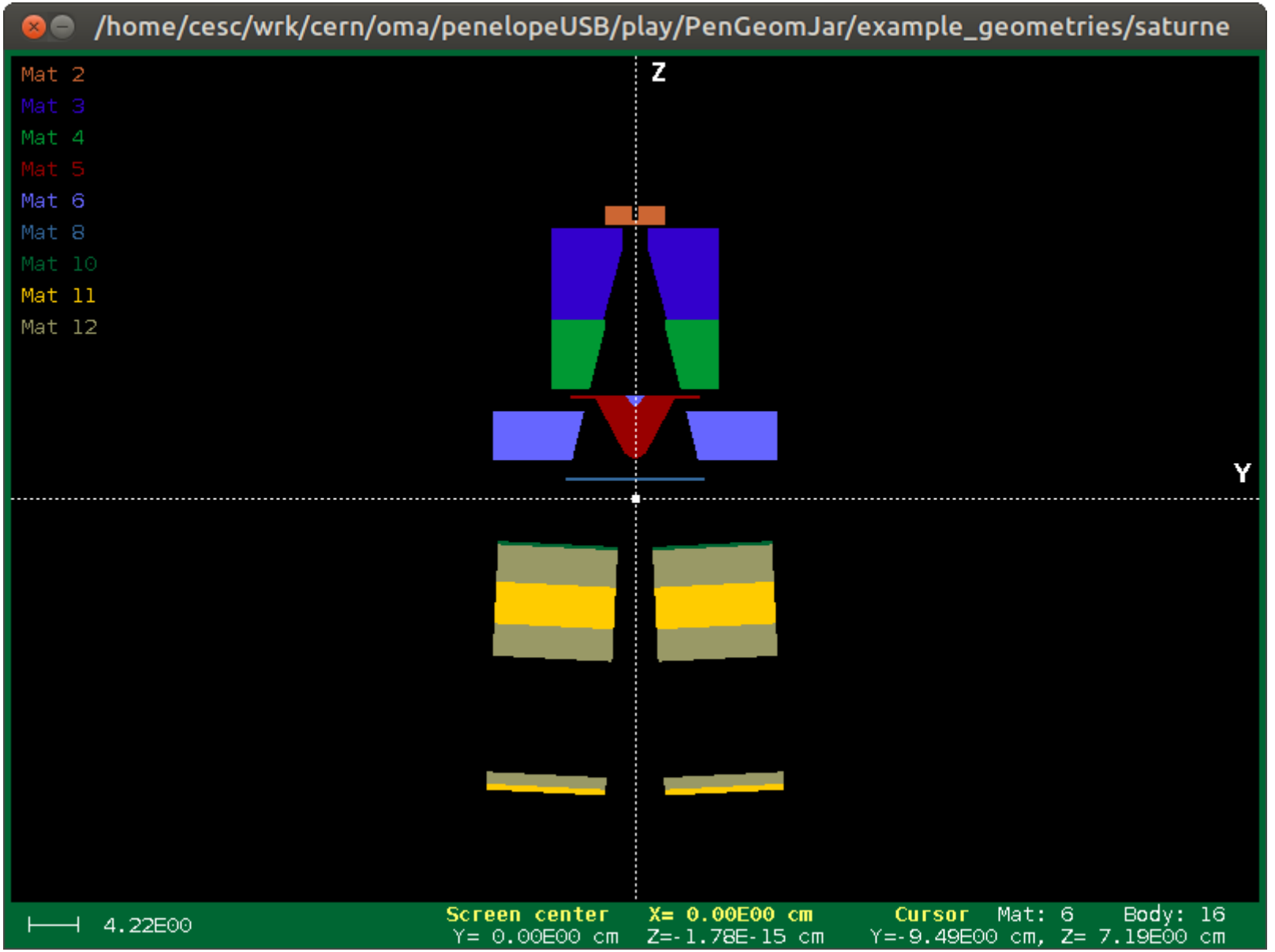
Omega= 90.00° Theta= 0.00° Phi= 0.00°
Last clicked position info.
Mat: 4 Body: 154 Surf: 127

PenGeomJar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Mat 2
Mat 3
Mat 4
Mat 5
Mat 6
Mat 8
Mat 10
Mat 11
Mat 12
Z
Y
4.22E00
Screen center X= 0.00E00 cm
Y= 0.00E00 cm Z=-1.78E-15 cm
Cursor Mat: 6 Body: 16
Y=-9.49E00 cm, Z= 7.19E00 cm

GUI coming soon….

Geometry / Input / Output

7) Obtaining the software

Official PENELOPE distribution

https://www.oecd-nea.org/tools/abstract/detail/nea-1525

Computer Programs
NEA-1525 PENELOPE2014.

NEA-1525 PENELOPE2014.

PENELOPE2014, A Code System for Monte-Carlo Simulation of Electron and Photon Transport

1. NAME OR DESIGNATION OF PROGRAM

[top]

PENELOPE2014

2. COMPUTERS

[top]

To submit a request, click below on the link of the version you wish to order. Rules for end-users are available here.

Program name	Package id	Status	Status date
PENELOPE2014	NEA-1525/22	Tested	11-MAY-2015

Machines used:

Package ID	Orig. computer	Test computer
NEA-1525/22	Linux-based PC,PC Windows,UNIX W.S.	PC Windows

3. DESCRIPTION OF PROGRAM OR FUNCTION

[top]

PENELOPE performs Monte Carlo simulation of coupled electron-photon transport in arbitrary materials and complex quadric geometries. A mixed procedure is used for the simulation of electron and positron interactions (elastic scattering, inelastic scattering and bremsstrahlung emission), in which 'hard' events (i.e. those with deflection angle and/or energy

Official PENGEOM distribution

https://www.oecd-nea.org/tools/abstract/detail/nea-1886/

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Computer Programs
NEA-1886 PENGEOM.

NEA-1886 PENGEOM.

last modified: 08-JAN-2016 | catalog | categories | new | search | RSS

PENGEOM, tools for handling complex quadric geometries in Monte Carlo simulations of radiation transport

NAME, COMPUTER, PROBLEM, SOLUTION, RESTRICTIONS, CPU, FEATURES, AUXILIARIES, STATUS, REFERENCES, REQUIREMENTS, LANGUAGE, OPERATING SYSTEM, AUTHOR, MATERIAL, CATEGORIES

1. NAME OR DESIGNATION OF PROGRAM

[top

PENGEOM

2. COMPUTERS

[top

To submit a request, click below on the link of the version you wish to order. Rules for end-users are available here.

Program name	Package id	Status	Status date
PENGEOM	NEA-1886/02	Tested	08-JAN-2016

Machines used:

Package ID	Orig. computer	Test computer
NEA-1886/02	MAC,Linux-based PC,PC Windows	PC Windows

3. DESCRIPTION OF PROGRAM OR FUNCTION

[top

The Fortran subroutine package PENGEOM and the associated graphical user interface PenGeomJar constitute a complete set of tools for handling complex quadric geometries in Monte Carlo simulations of radiation transport. The material structure where radiation propagates is assumed to consist of homogeneous bodies limited by quadric surfaces. The PENGEOM

Summary

1) Elastic scattering of electrons and positrons.
ELSEPA (2005) → ICRU77 (2007) → NIST SRD64 (2016).

2) Cross sections for atomic inner-shell ionization by e-/e+ impact.
Bote & Salvat (2008) → J Phys Chem Ref Dat (2014) → NIST164 (2015).

3) Photoelectric absorption: Sabbatucci & Salvat (2016).

4) PENH: proton transport
Class II, EM interactions only, elastic scattering (screened point nucleus),
Nuclear elastic scattering and nuclear recoil effects under dev.

5) Radioactive sources (Garcia-Toraño 2017)

6) PenGeom