Radiation interaction with matter

Giancarlo Pepponi
Fondazione Bruno Kessler
MNF – Micro Nano Facility

MAUD school 2015
Trento, Italy

Radiation – x-rays (photons) , neutrons, electrons

	Planck / Einstein	De Broglie
Wave – particle duality	$E = h\nu$	$\lambda = \frac{h}{p}$

---

x-rays **photons**	electromagnetic radiation 0 rest mass $c = \lambda\nu$	$\lambda = \frac{hc}{E}$
neutrons	neutral particles 1.675e-27 kg 939.6 MeV/c2	$E_k = \frac{1}{2}mv^2 = \frac{p^2}{2m}$ $\lambda = \frac{h}{mv}$
electrons	charged particles 9.11e−31 kg 511.0 keV/c2	$E_k = eV = \frac{1}{2}mv^2 = \frac{p^2}{2m}$ $\lambda = \frac{h}{\sqrt{2meV}} \frac{1}{\sqrt{1+\frac{eV}{2mc^2}}}$

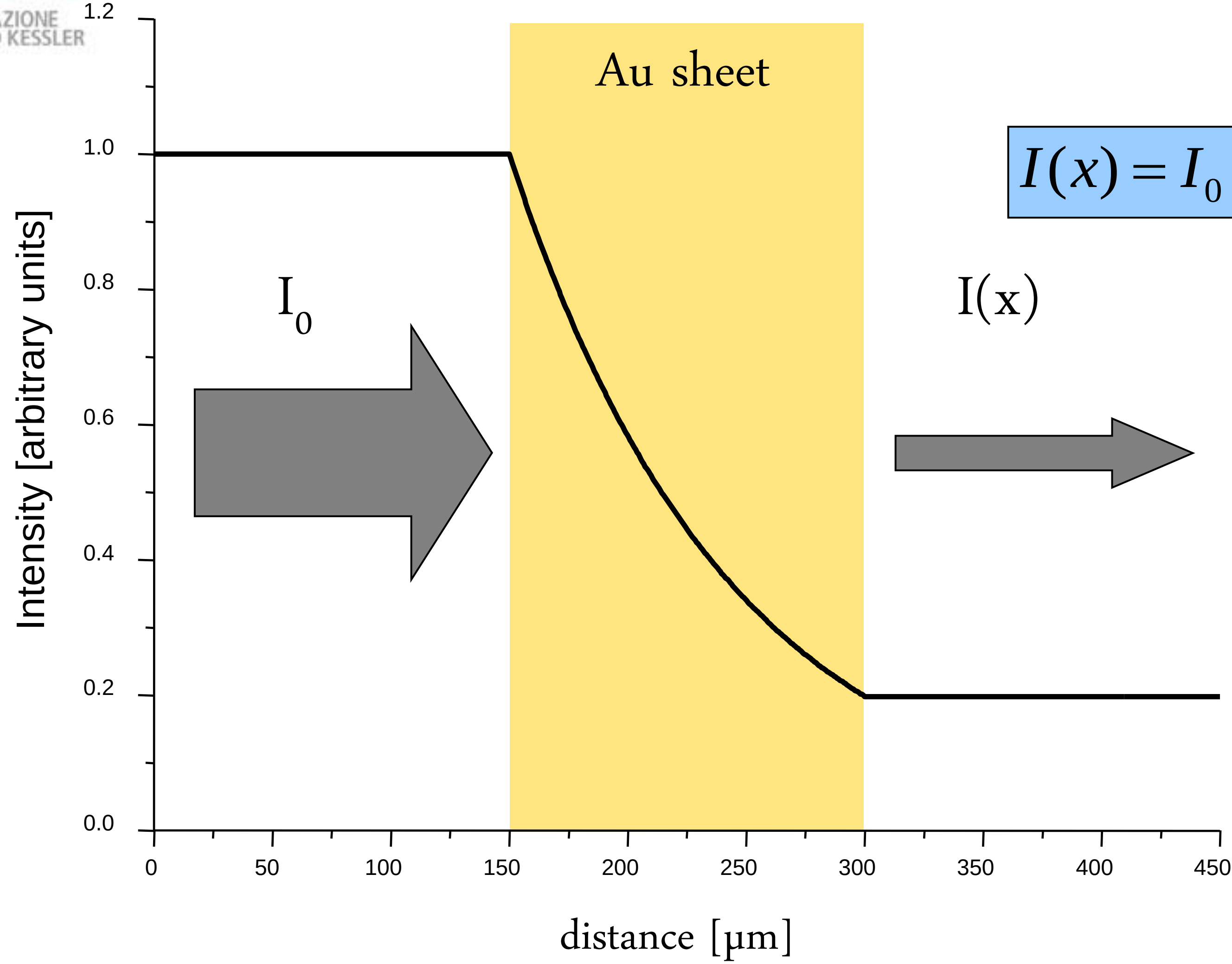
Radiation – x-rays (photons) , neutrons, electrons

	interaction type	interaction partners
x-rays photons	dipole photoelectric absorption	electrons atoms/electrons
neutrons	strong force magnetic neutron capture	nuclei unpaired electrons nuclei
electrons	Coulomb force	electrons, nuclei

Radiation – x-rays (photons) , neutrons, electrons

		energy	wavelength	velocity	temperature
x-rays photons	CuKa1 MoKa1	8.048 keV 17.479 keV	1.54 A 0.71 A		
neutrons	thermal cold	25 meV 6.6 meV	1.8 A 3.5 A	2200 m/s 1127 m/s	293.6 K 77 K
electrons	SEM TEM	20 keV 200 keV	0.122 A 0.025 A		

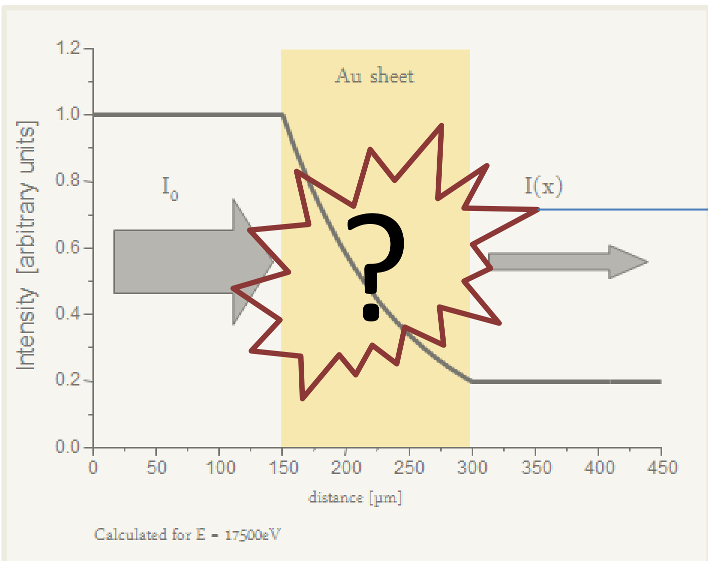
Radiation – attenuation - Beer Lambert law



$$I(x) = I_0 \exp(-\mu x)$$

Calculated for X-Rays E = 17500eV

Radiation – attenuation - Beer Lambert law



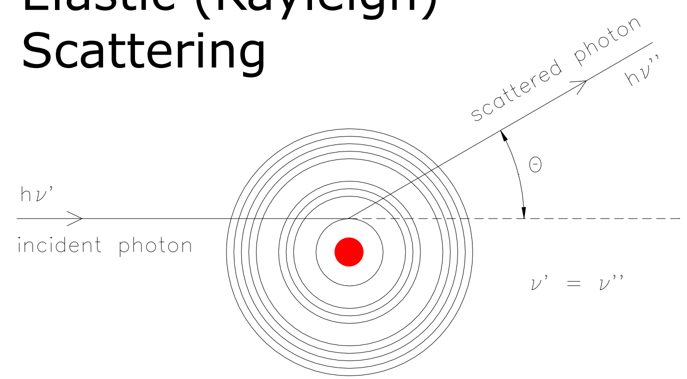
Scattering
(elastic, inelastic)
Absorption

$$I(x) = I_0 \exp(-\mu x)$$

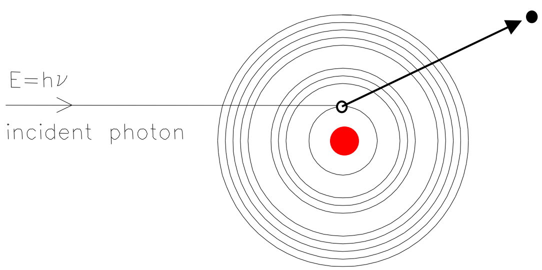
$$\mu = \mu_a + \mu_s$$

Attenuation X-Rays : microscopic view

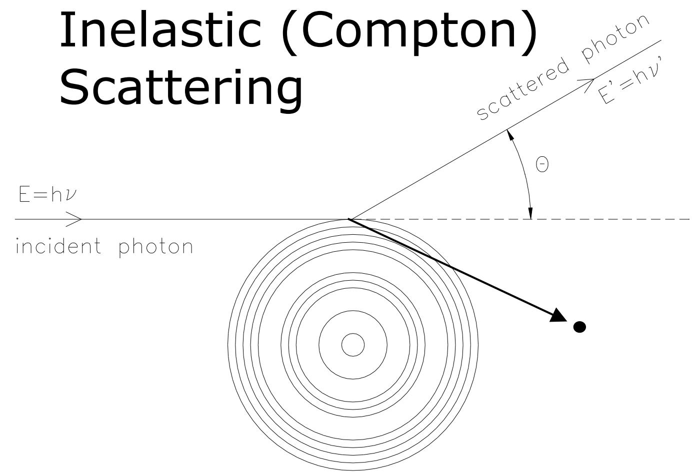
Elastic (Rayleigh) Scattering



Photoelectric absorption



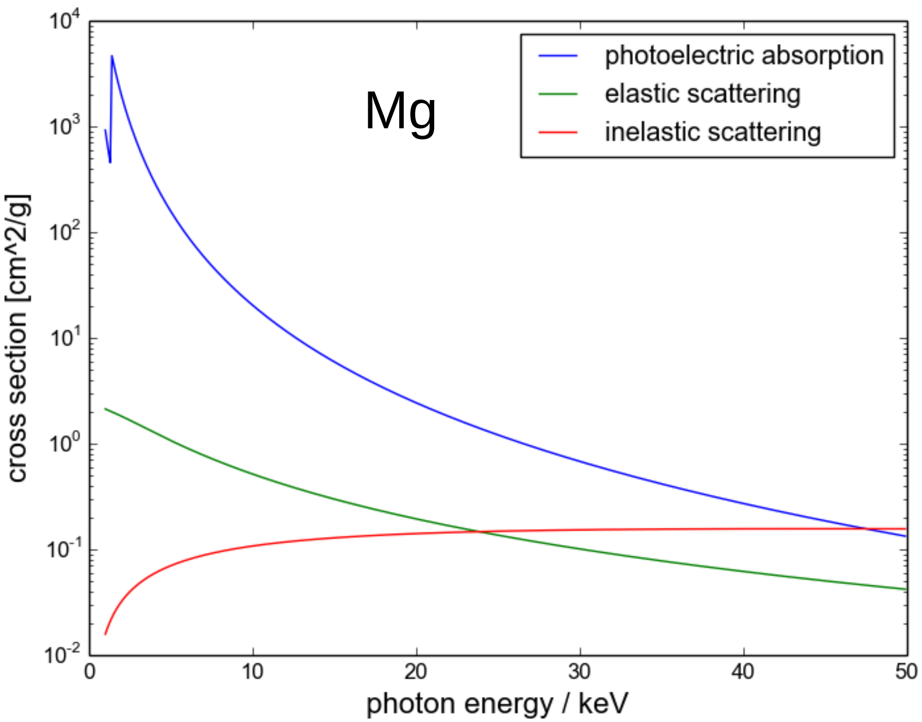
Inelastic (Compton) Scattering

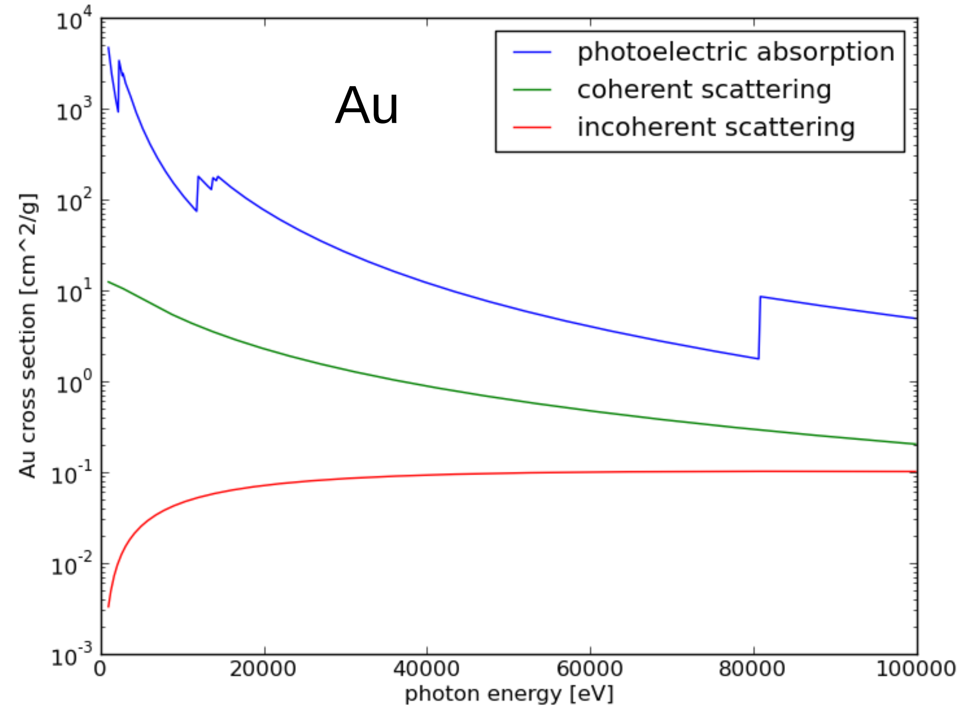


X-Rays cross section magnitude

$$I(x) = I_0 \exp(-\mu x)$$

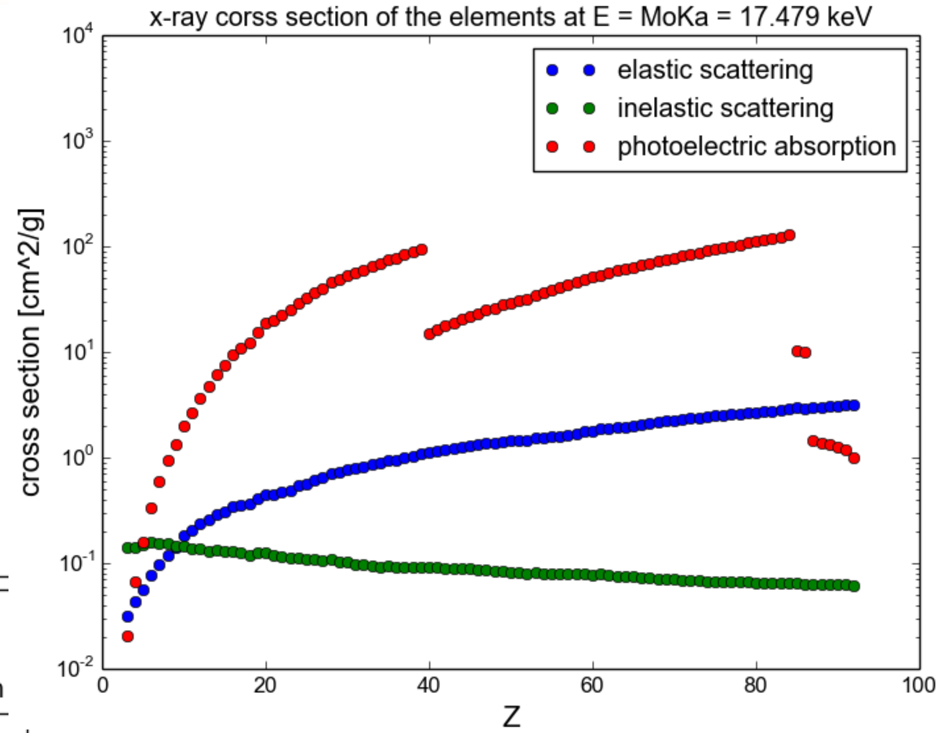
$$\mu = \sigma_c + \sigma_i + \tau$$



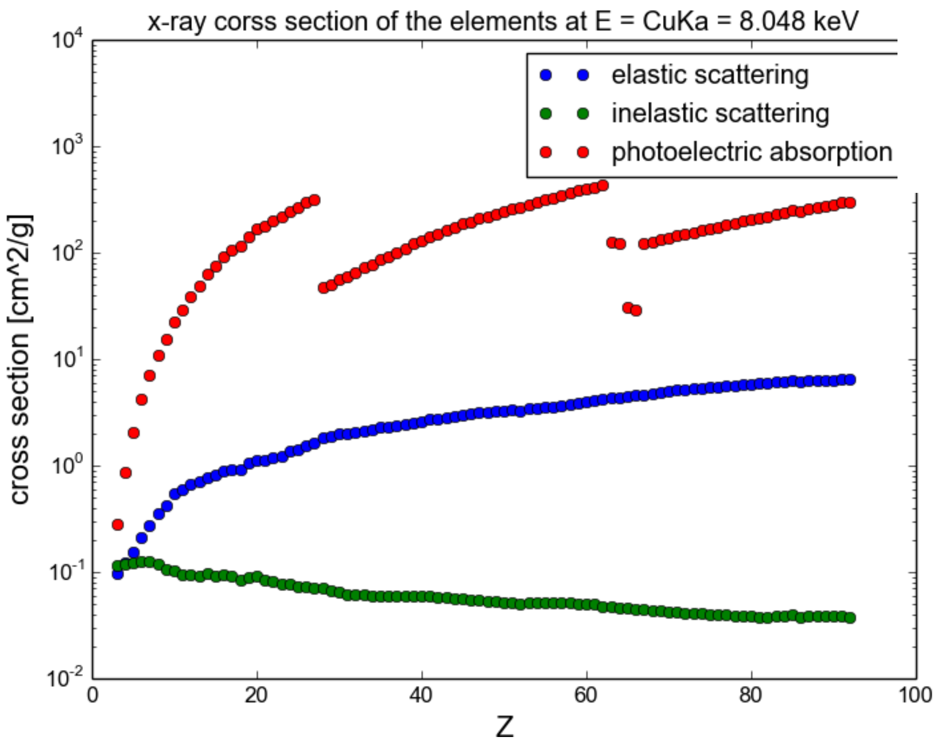


data from:
H. Ebel, R. Svagera, M. F. Ebel, A. Shaltout and J. H. Hubbell,
Numerical description of photoelectric absorption coefficients for fundamental parameter programs,
X-Ray Spectrometry, 32, 442–451 (2003)

X-Rays

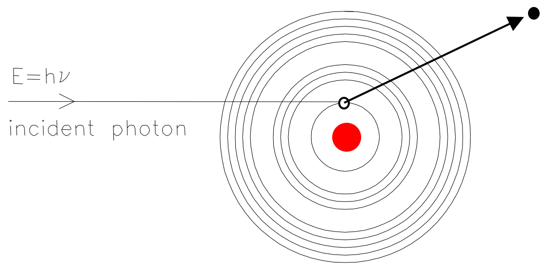


x-ray corss section of the elements at E = MoKa = 17.479 keV
elastic scattering
inelastic scattering
photoelectric absorption
cross section [cm^2/g]
Z



x-ray corss section of the elements at E = CuKa = 8.048 keV
elastic scattering
inelastic scattering
photoelectric absorption
cross section [cm^2/g]
Z

Atomic binding energies, electron energy levels

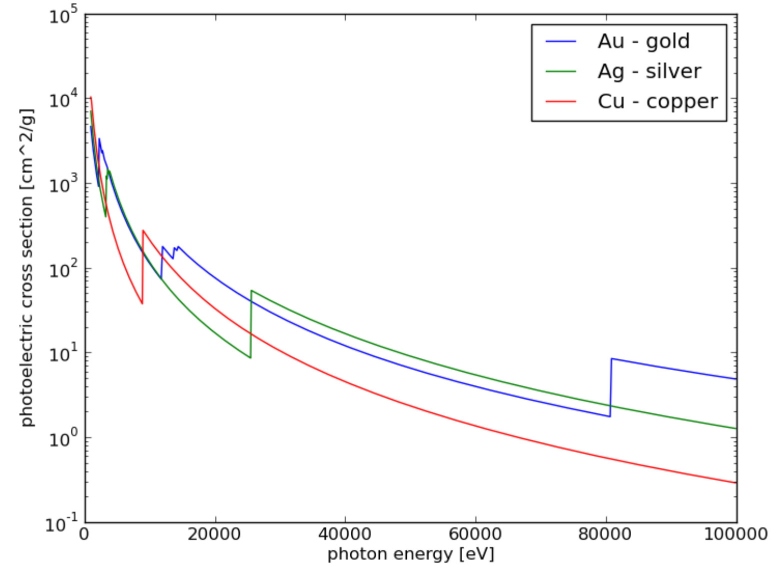


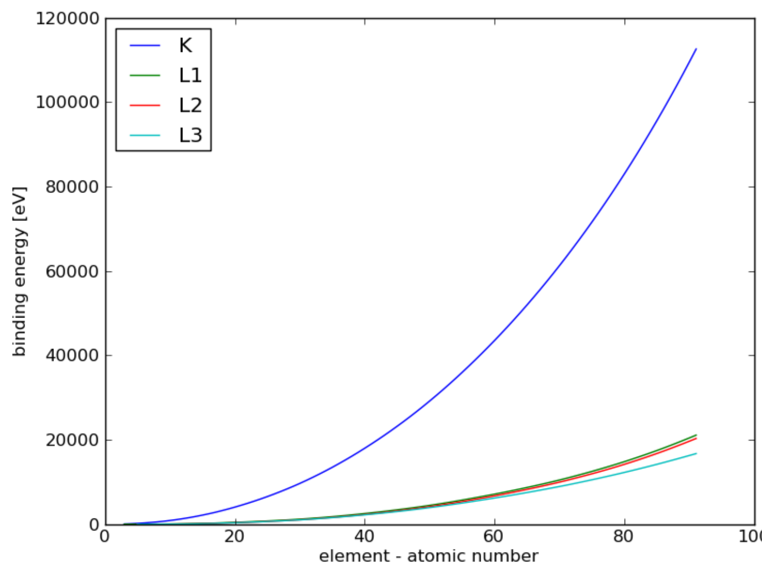
Absorption edges
Electron energy levels
Shells

shell	n	l	j	spin sign	max number of electrons
K	1	0	0.5	1	2
L1	2	0	0.5	1	2
L2	2	1	0.5	-1	2
L3	2	1	1.5	1	4
M1	3	0	0.5	1	2
M2	3	1	0.5	-1	2
M3	3	1	1.5	1	4
M4	3	2	1.5	-1	4
M5	3	2	2.5	1	6

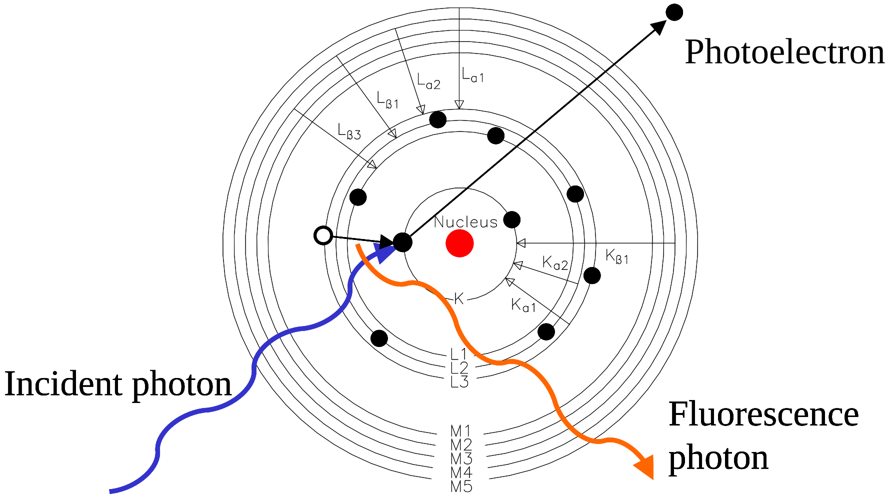
Z	shell	energy_eV	jump	level_width_eV
79	K	80724.9	4.874	52.1
79	L1	14352.8	1.15567	9.8
79	L2	13733.6	1.4	5.53
79	L3	11918.7	2.55	5.54
79	M1	3424.9	1.04	15.0
79	M2	3147.8	1.058	9.5
79	M3	2743.0	1.15776	8.5
79	M4	2291.1	1.07	2.18
79	M5	2205.7	1.092	2.18

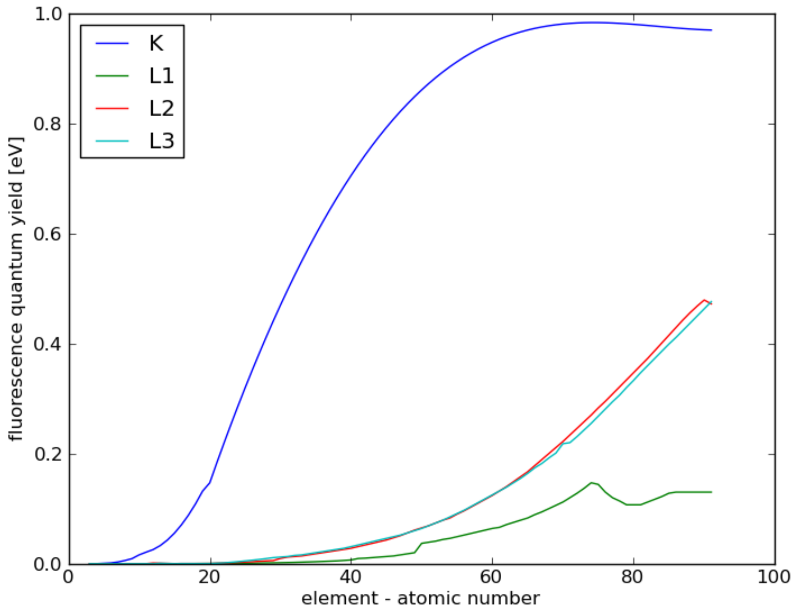
www.txrf.org/xraydata

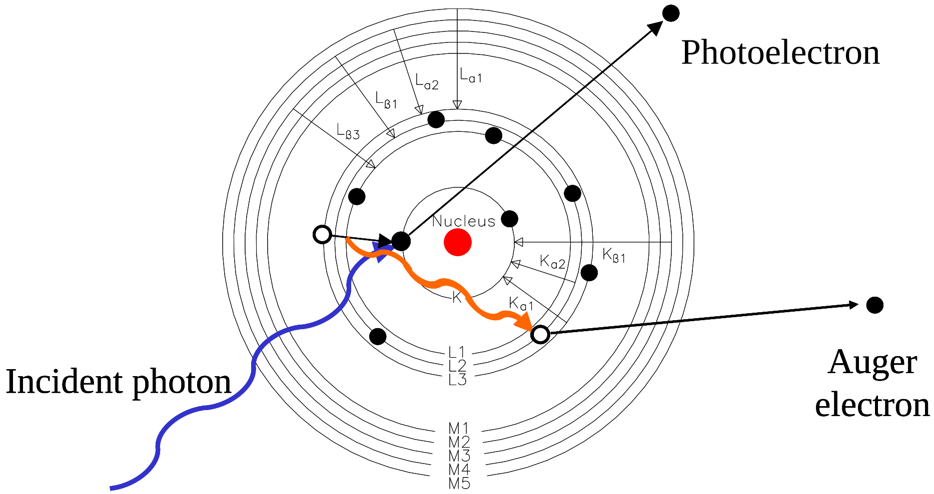




Secondary effects – fluorescence vs Auger





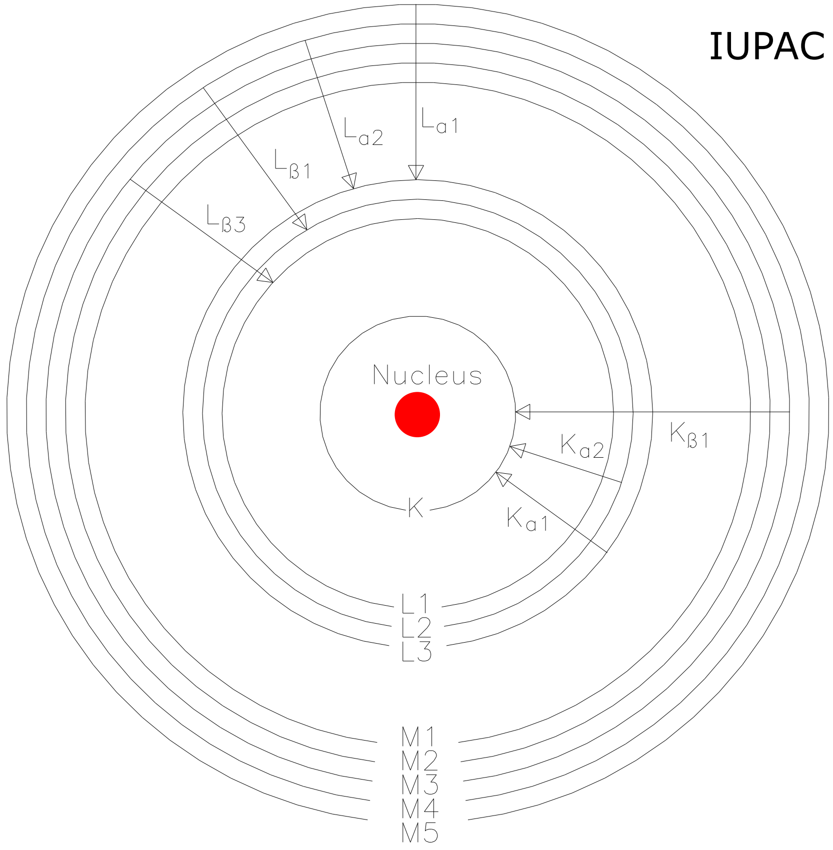


data from:
M. O. Krause,
J. Phys. Chem. Ref. Data 8 (1979) 307

X-Ray Fluorescence – characteristic lines

Siegbahn = Manne Siegbahn (swedish physicist)
Nobel Prize in Physics in 1924

IUPAC = International Union of Pure and Applied Chemistry

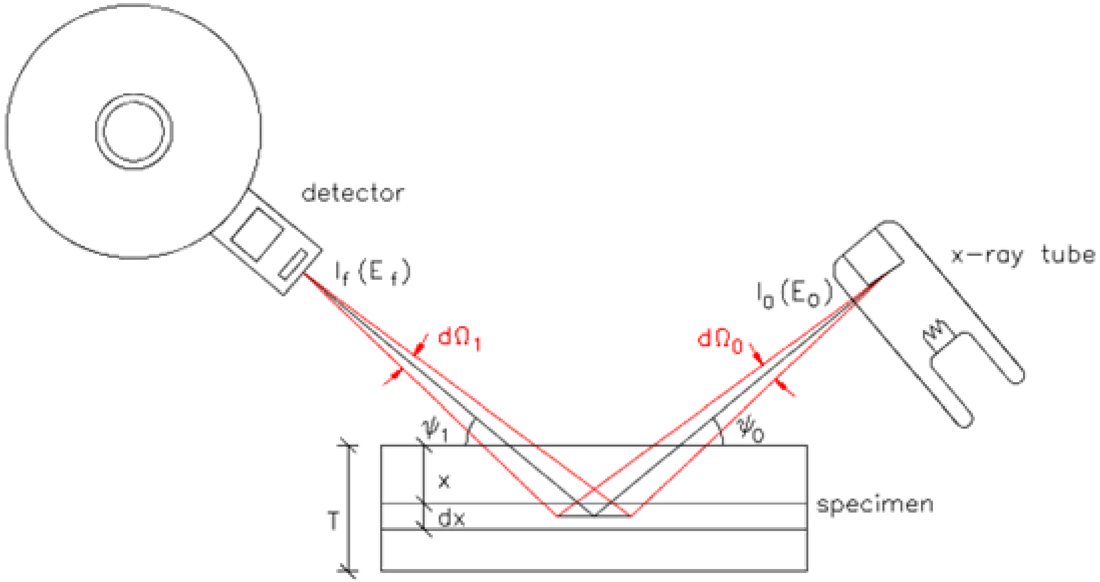


Siegbahn	IUPAC	Siegbahn	IUPAC
$K\alpha_1$	K-L3	$L\alpha_1$	L3-M5
$K\alpha_2$	K-L2	$L\alpha_2$	L3-M4
$K\beta_1$	K-M3	$L\beta_1$	L2-M4
$K\beta_2$	K-N2,N3	$L\beta_2$	L3-N5
$K\beta_3$	K-M2	$L\beta_3$	L1-M3
		$L\beta_4$	L1-M2

Germanium

Line	Energy [keV]	Probability
$K\alpha_1$	9.887	0.57380
$K\alpha_2$	9.856	0.29550
$K\beta_1$	10.983	0.08470
$K\beta_2$	11.103	0.00280
$K\beta_3$	10.978	0.04320

X-Ray Fluorescence – intensity - Sherman equation



$$I_0\, G_0\, G_1$$

geometrical factors and primary flux form the element independent proportionality constant

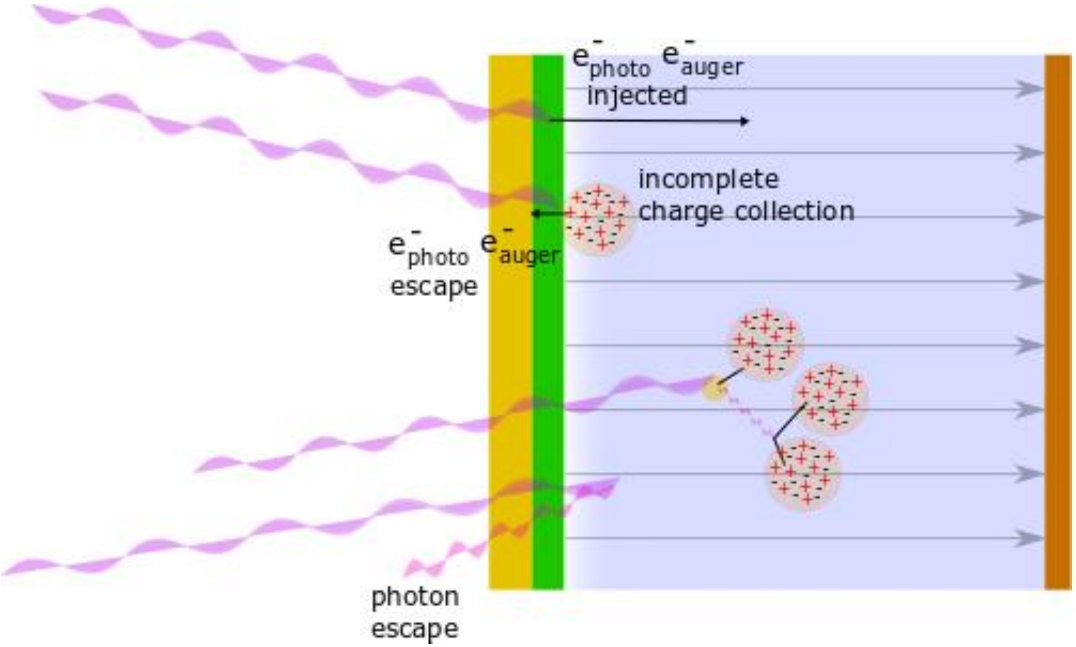
$$dI_{\zeta jk} \propto \underbrace{e^{-\mu_{s,E_0}\frac{z}{\sin\phi_i}}}_{1.}\ \underbrace{W_\zeta \left(\frac{\tau_j}{\rho}\right)_{\zeta E_0} \rho_s dz}_{2.} \cdot \underbrace{\omega_{\zeta j}}_{3.}\ \underbrace{p_{\zeta jk}}_{4.}\ \underbrace{e^{-\mu_{s,E_{\zeta jk}}\frac{z}{\sin\phi_f}}}_{5.}\ \underbrace{\epsilon_{E_{\zeta jk}}}_{6.}$$

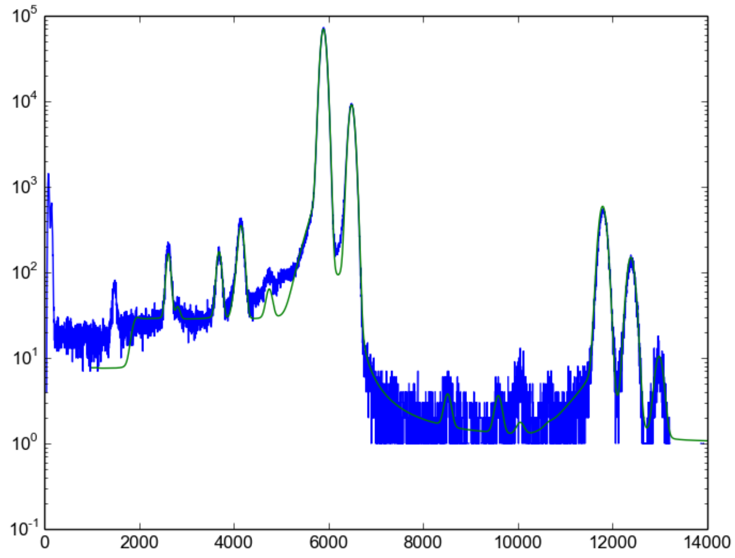
1. attenuation to depth z
2. photoelectric absorption in layer dz
3. fluorescence yield
4. transition probability (relative intensity of lines in shell)
5. attenuation to the detector
6. detector efficiency

EDS detector

$$\epsilon_{E_{\zeta j k}}$$

detector efficiency + response

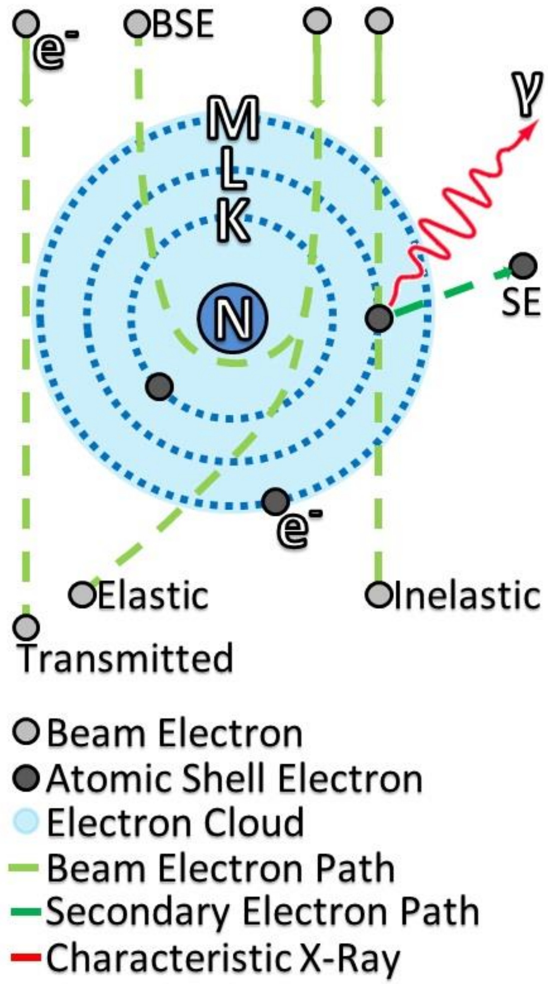




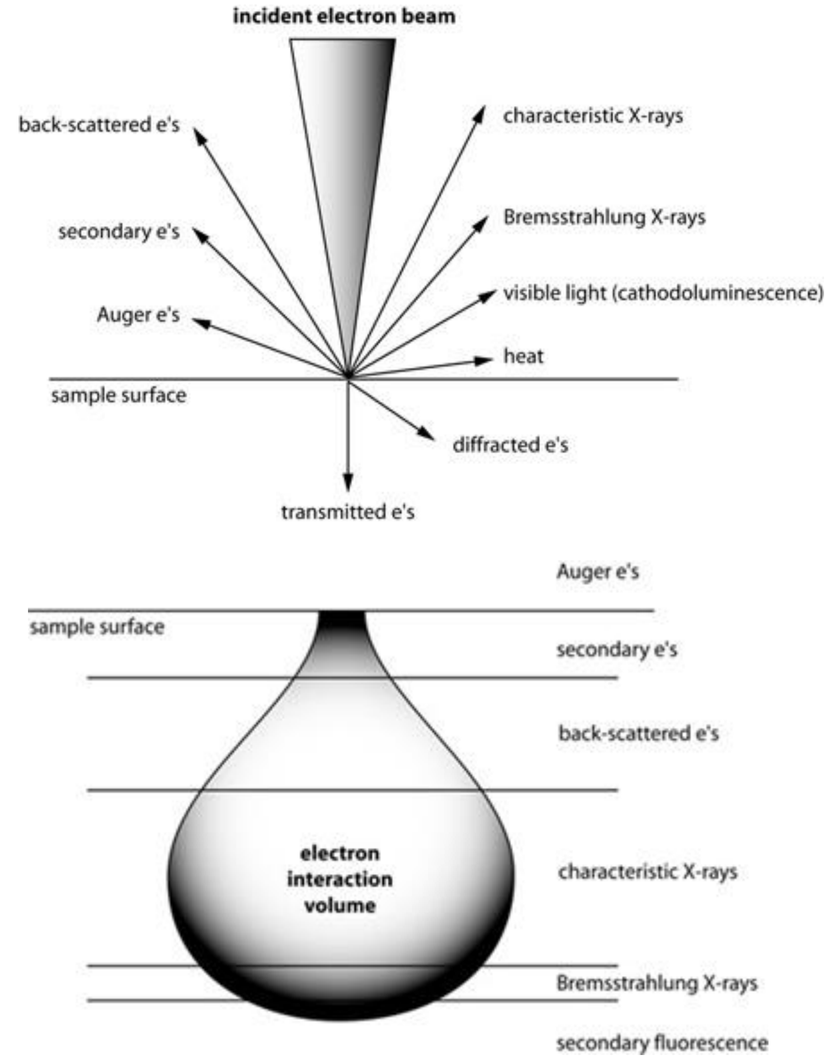
Modelling the response function of energy dispersive X-ray spectrometers with silicon detectors

F. Scholze, and M. Procop

Electrons interaction with matter

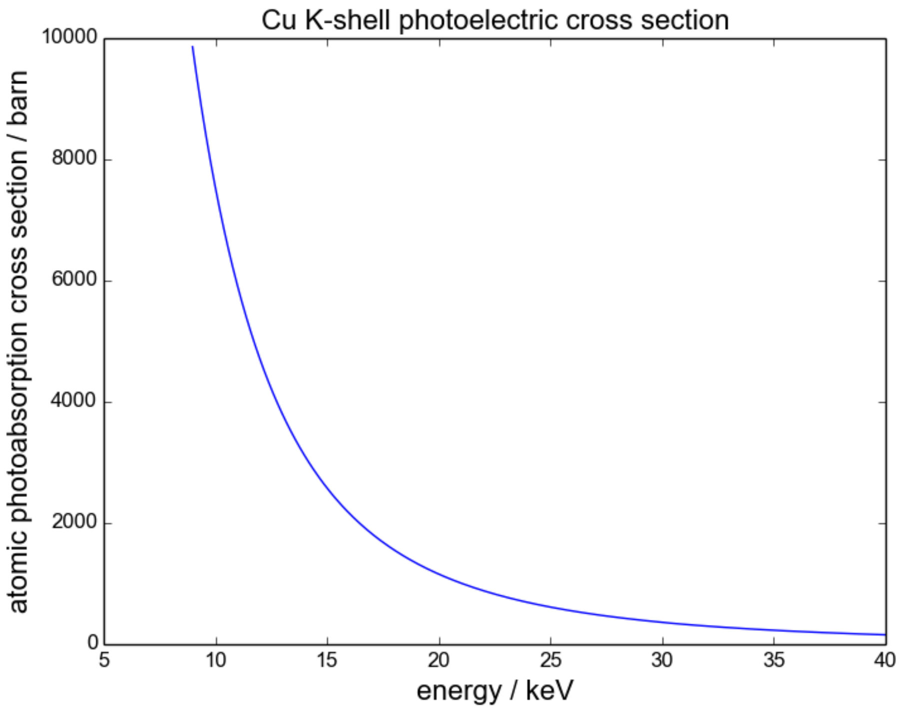


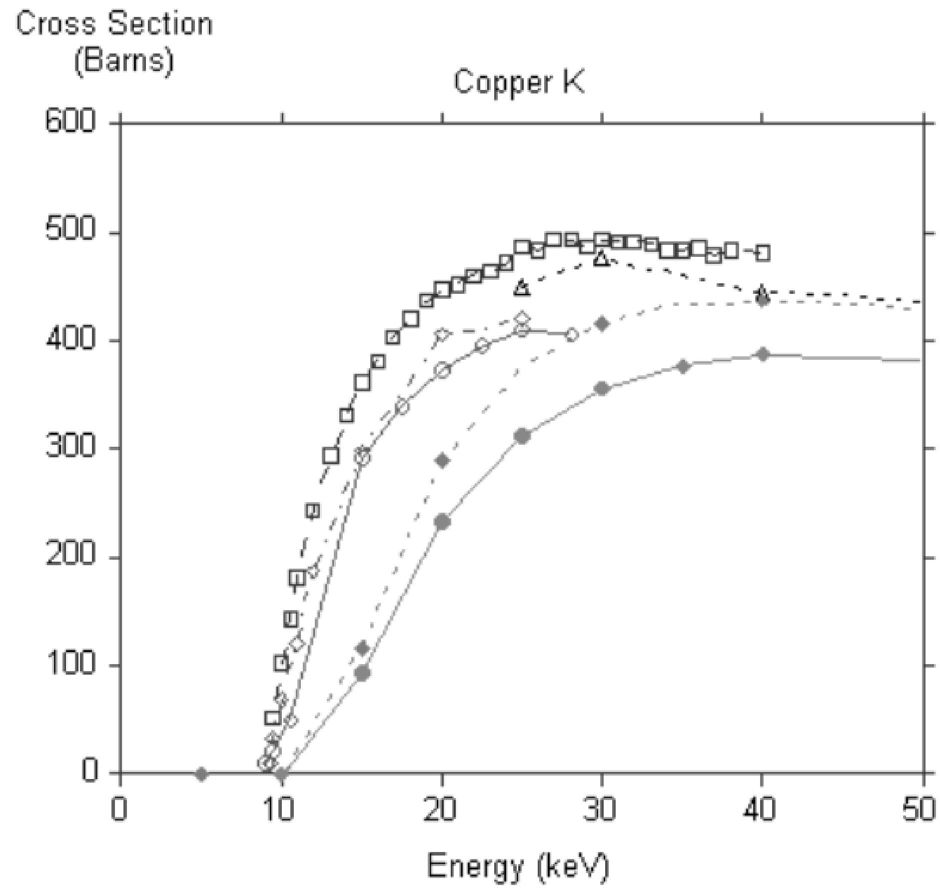
https://en.wikipedia.org/wiki/Electron_scattering

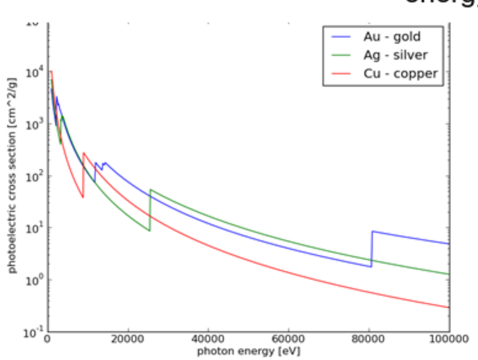


http://serc.carleton.edu/research_education/geochemsheets/electroninteractions.html

Inner shell ionization cross section: x-rays vs electrons







Volume 107, Number 6, November–December 2002
Journal of Research of the National Institute of Standards and Technology

Neutrons interaction with matter

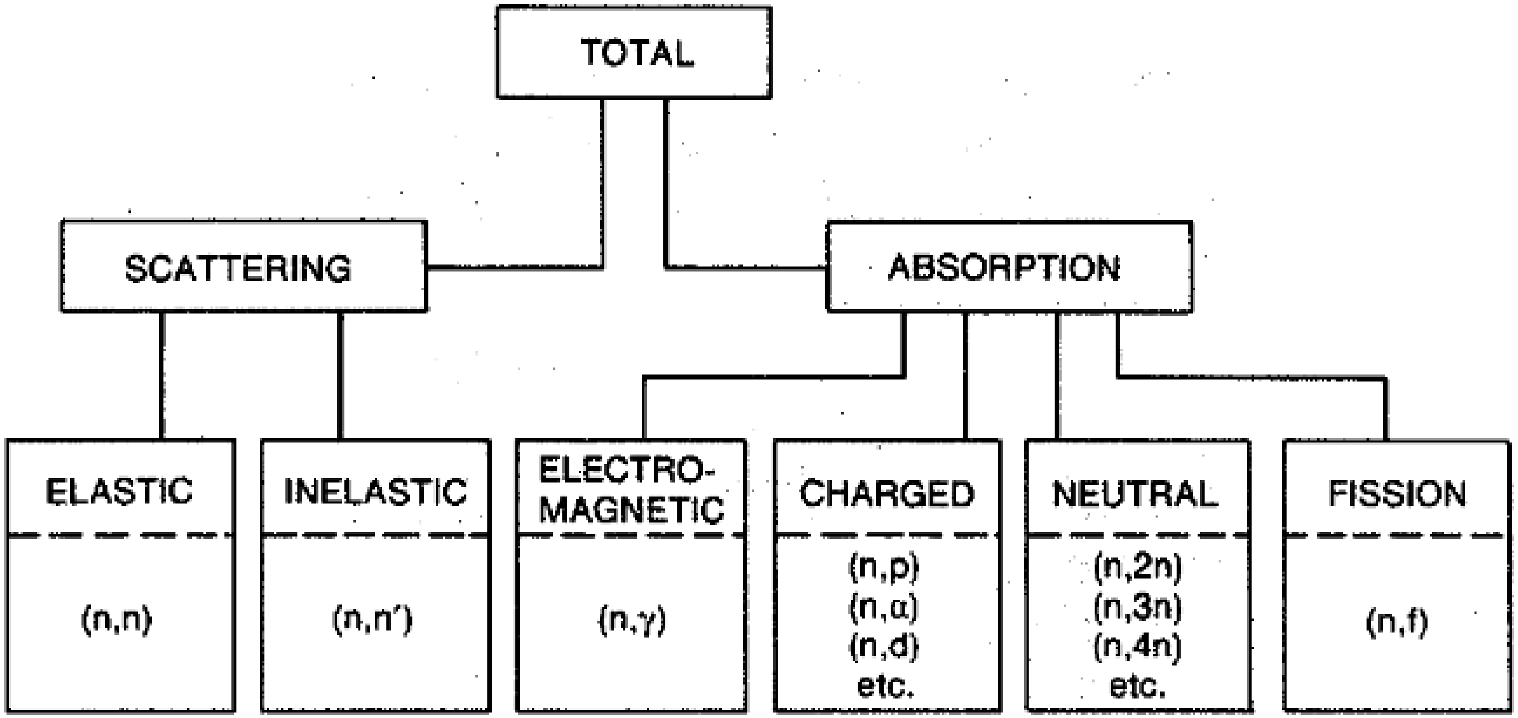
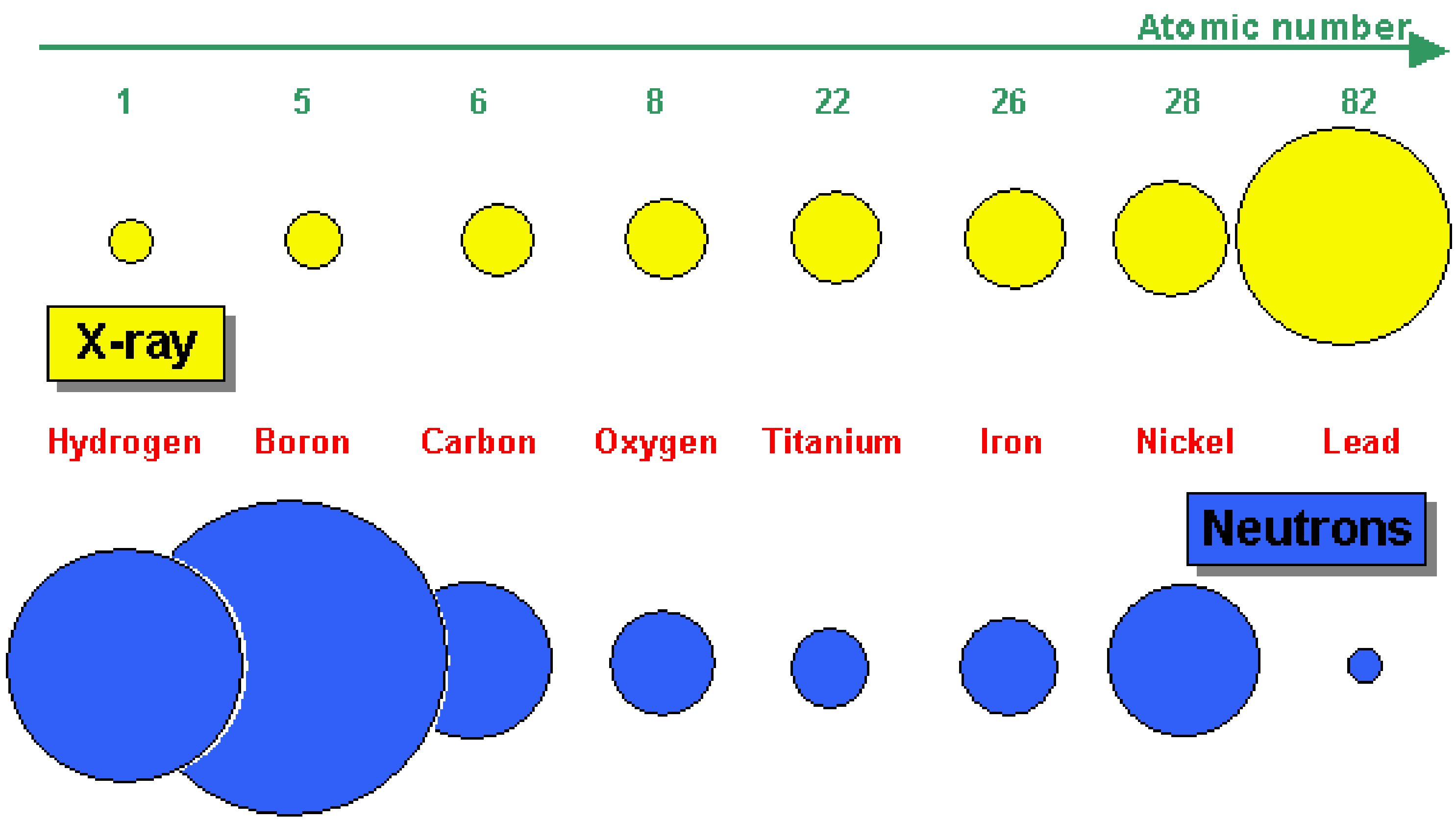


Fig. 12.2 *Various categories of neutron interactions. The letters separated by commas in the parentheses show the incoming and outgoing particles.*

http://www.uio.no/studier/emner/matnat/fys/FYS-KJM4710/h14/timeplan/neutron_chapter.pdf

Cross section : x-rays vs neutrons



https://www.psi.ch/niag/comparison-to-x-ray

Cross section : x-rays vs neutrons

Attenuation coeffitients for thermal neutrons [cm^{-1}]

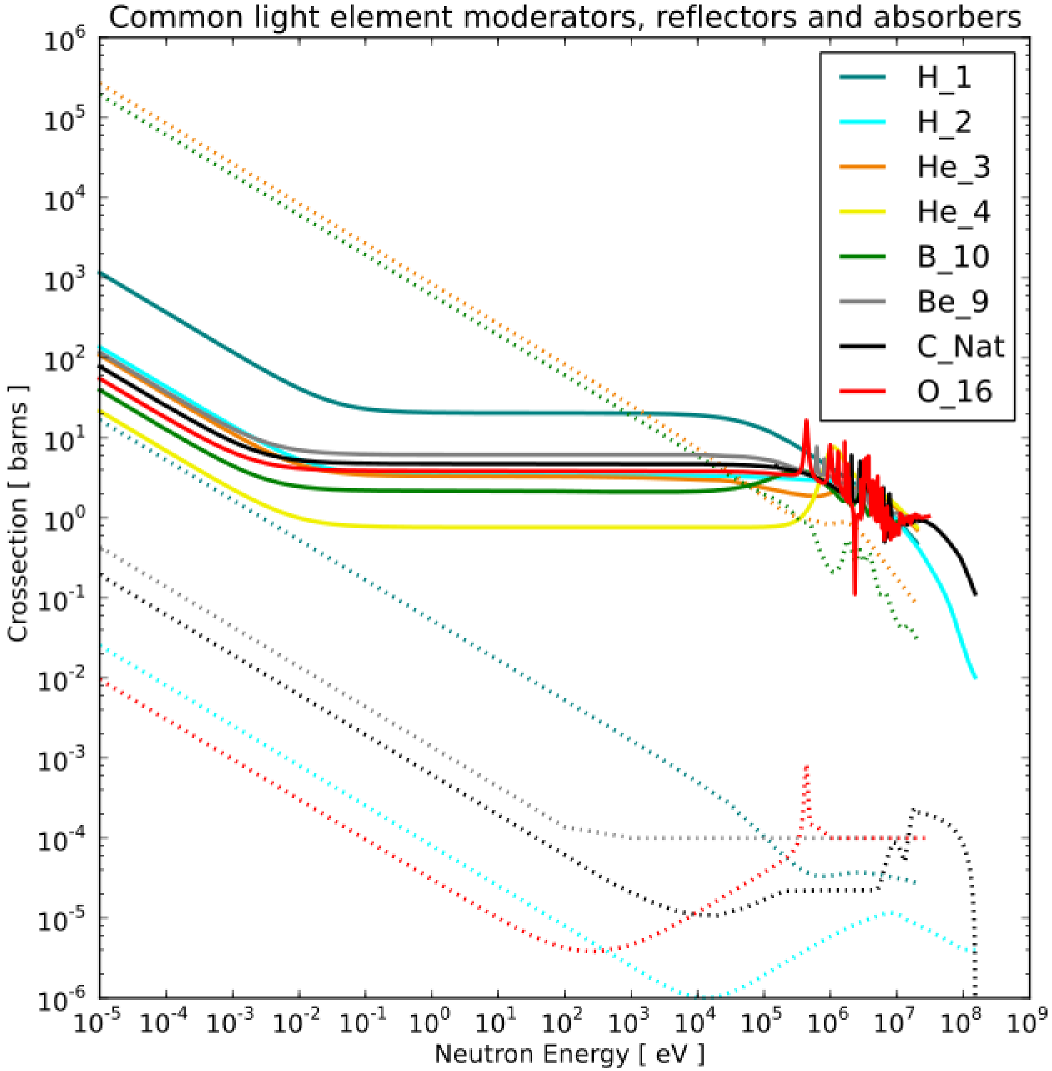
1a	2a	3b	4b	5b	6b	7b	8			1b	2b	3a	4a	5a	6a	7a	0
H 3.44																	He 0.02
Li 3.30	Be 0.79											B 101.60	C 0.56	N 0.43	O 0.17	F 0.20	Ne 0.10
Na 0.09	Mg 0.15											Al 0.10	Si 0.11	P 0.12	S 0.06	Cl 1.33	Ar 0.03
K 0.06	Ca 0.08	Sc 2.00	Ti 0.60	V 0.72	Cr 0.54	Mn 1.21	Fe 1.19	Co 3.92	Ni 2.05	Cu 1.07	Zn 0.35	Ga 0.49	Ge 0.47	As 0.67	Se 0.73	Br 0.24	Kr 0.61
Rb 0.08	Sr 0.14	Y 0.27	Zr 0.29	Nb 0.40	Mo 0.52	Tc 1.76	Ru 0.58	Rh 10.88	Pd 0.78	Ag 4.04	Cd 115.11	In 7.58	Sn 0.21	Sb 0.30	Te 0.25	I 0.23	Xe 0.43
Cs 0.29	Ba 0.07	La 0.52	Hf 4.99	Ta 1.49	W 1.47	Re 6.85	Os 2.24	Ir 30.46	Pt 1.46	Au 6.23	Hg 16.21	Tl 0.47	Pb 0.38	Bi 0.27	Po	At	Rn
Fr	Ra 0.34	Ac	Rf	Ha													
*Lanthanides	Ce 0.14	Pr 0.41	Nd 1.87	Pm 5.72	Sm 171.47	Eu 94.58	Gd 1479.04	Tb 0.93	Dy 32.42	Ho 2.25	Er 5.48	Tm 3.53	Yb 1.40	Lu 2.75			
**Actinides	Th 0.59	Pa 8.46	U 0.82	Np 9.80	Pu 50.20	Am 2.86	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

Attenuation coeffitients for X-ray [cm^{-1}] (150kV)

1a	2a	3b	4b	5b	6b	7b	8			1b	2b	3a	4a	5a	6a	7a	0
H 0.02																	He 0.02
Li 0.06	Be 0.22											B 0.28	C 0.27	N 0.11	O 0.16	F 0.14	Ne 0.17
Na 0.13	Mg 0.24											Al 0.38	Si 0.33	P 0.25	S 0.30	Cl 0.23	Ar 0.20
K 0.14	Ca 0.26	Sc 0.48	Ti 0.73	V 1.04	Cr 1.29	Mn 1.32	Fe 1.57	Co 1.78	Ni 1.96	Cu 1.97	Zn 1.64	Ga 1.42	Ge 1.33	As 1.50	Se 1.23	Br 0.90	Kr 0.73
Rb 0.47	Sr 0.86	Y 1.61	Zr 2.47	Nb 3.43	Mo 4.29	Tc 5.06	Ru 5.71	Rh 6.08	Pd 6.13	Ag 5.67	Cd 4.84	In 4.31	Sn 3.98	Sb 4.28	Te 4.06	I 3.45	Xe 2.53
Cs 1.42	Ba 2.73	La 5.04	Hf 19.70	Ta 25.47	W 30.49	Re 34.47	Os 37.92	Ir 39.01	Pt 38.61	Au 35.94	Hg 25.88	Tl 23.23	Pb 22.81	Bi 20.28	Po 20.22	At	Rn 9.77
Fr	Ra 11.80	Ac 24.47	Rf	Ha													
*Lanthanides	Ce 5.79	Pr 6.23	Nd 6.46	Pm 7.33	Sm 7.68	Eu 5.66	Gd 8.69	Tb 9.46	Dy 10.17	Ho 10.91	Er 11.70	Tm 12.49	Yb 9.32	Lu 14.07			
**Actinides	Th 28.95	Pa 39.65	U 49.08	Np	Pu	Am	Cm	Bk	Vf	Es	Fm	Md	No	Lr			

https://www.psi.ch/niag/comparison-to-x-ray

Neutron cross section

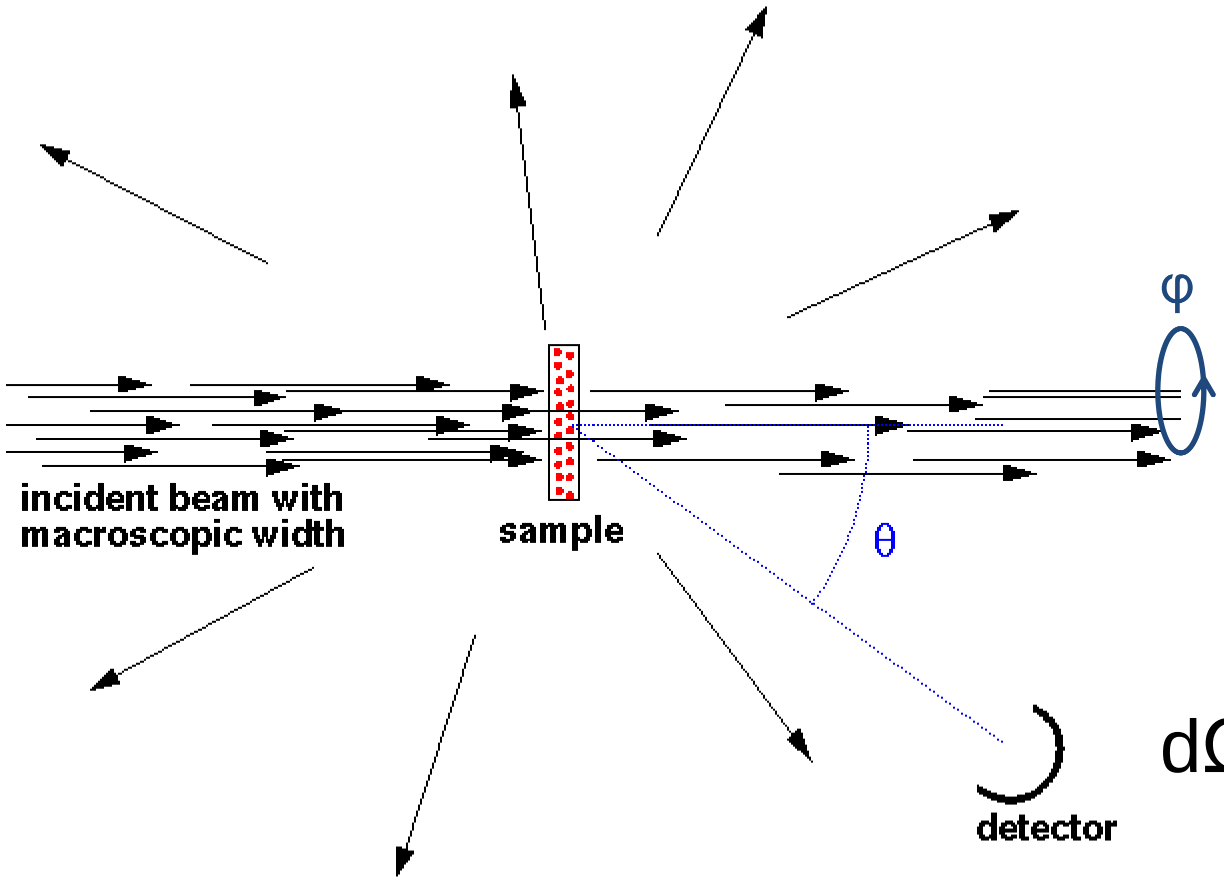


Scattering (full line) and absorption (dotted) cross sections of light element commonly used as neutron moderators, reflectors and absorbers, the data was obtained from database NEA N ENDF/B-VII.1 using JANIS software

https://en.wikipedia.org/wiki/Neutron_cross_section

Scattering - Differential cross section

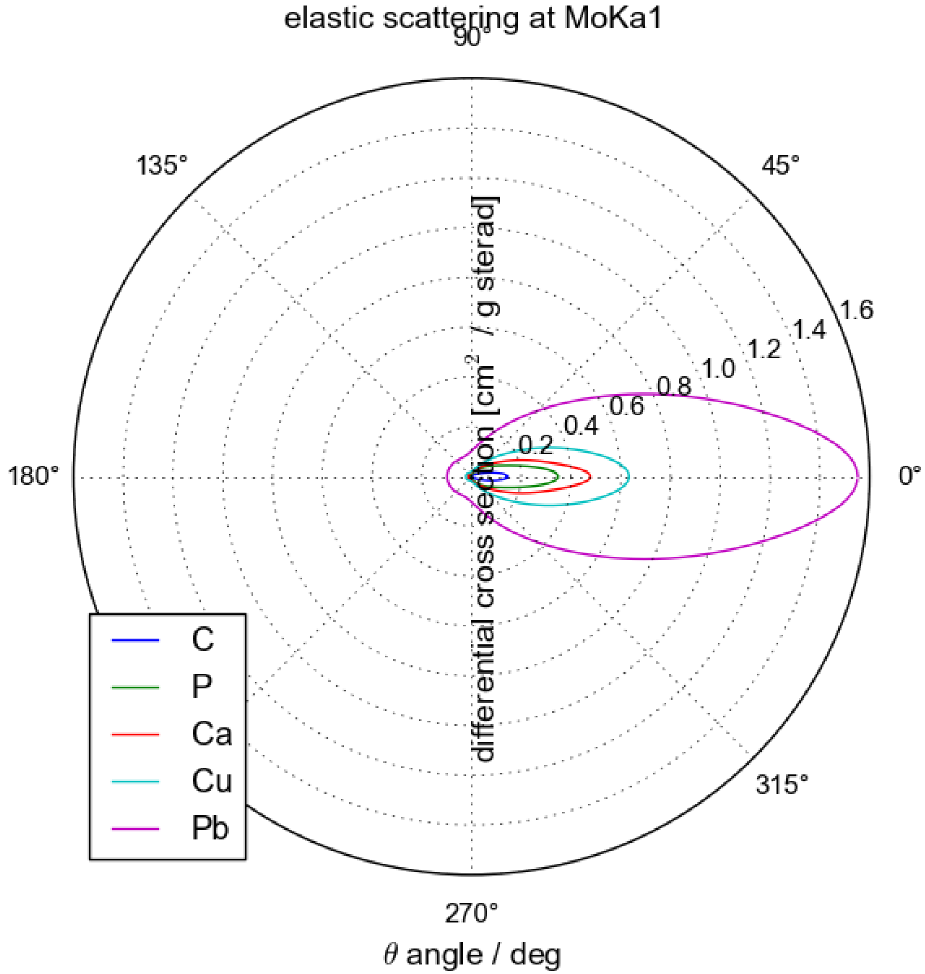
$$\frac{d\sigma}{d\Omega}$$

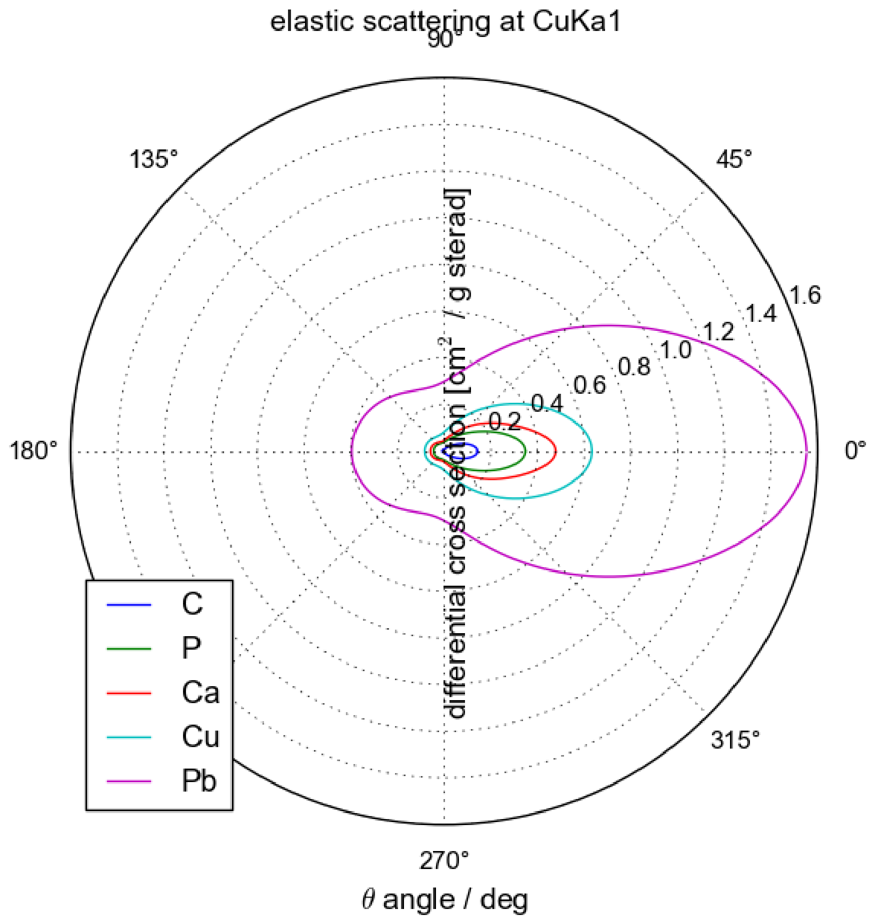


$$d\Omega = d\theta d\varphi$$

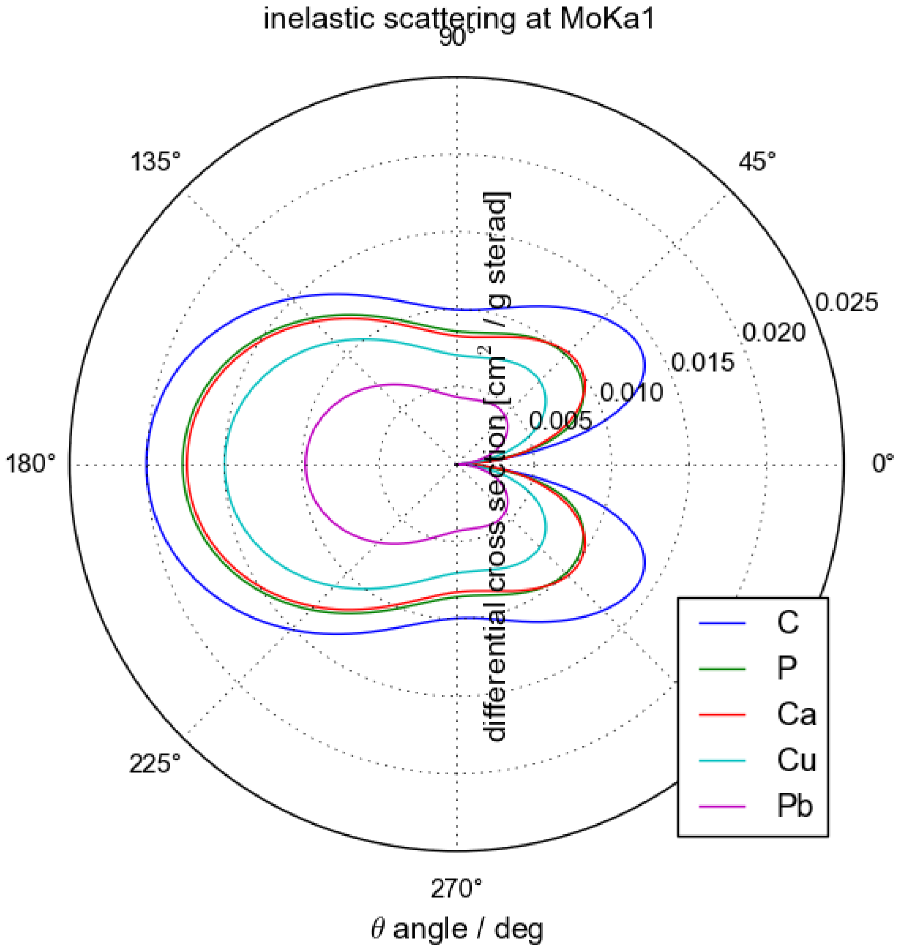
http://www.physics.csbsju.edu/QM/square.17.html

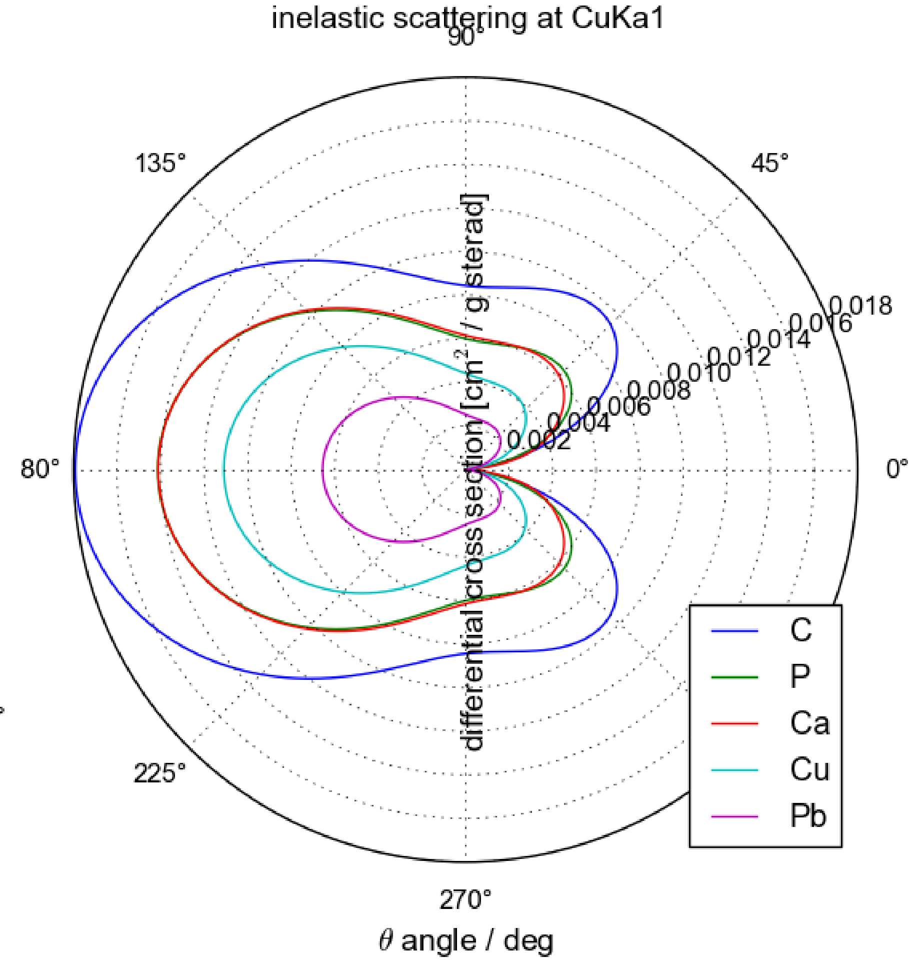
X-Rays - Differential cross section – elastic scattering



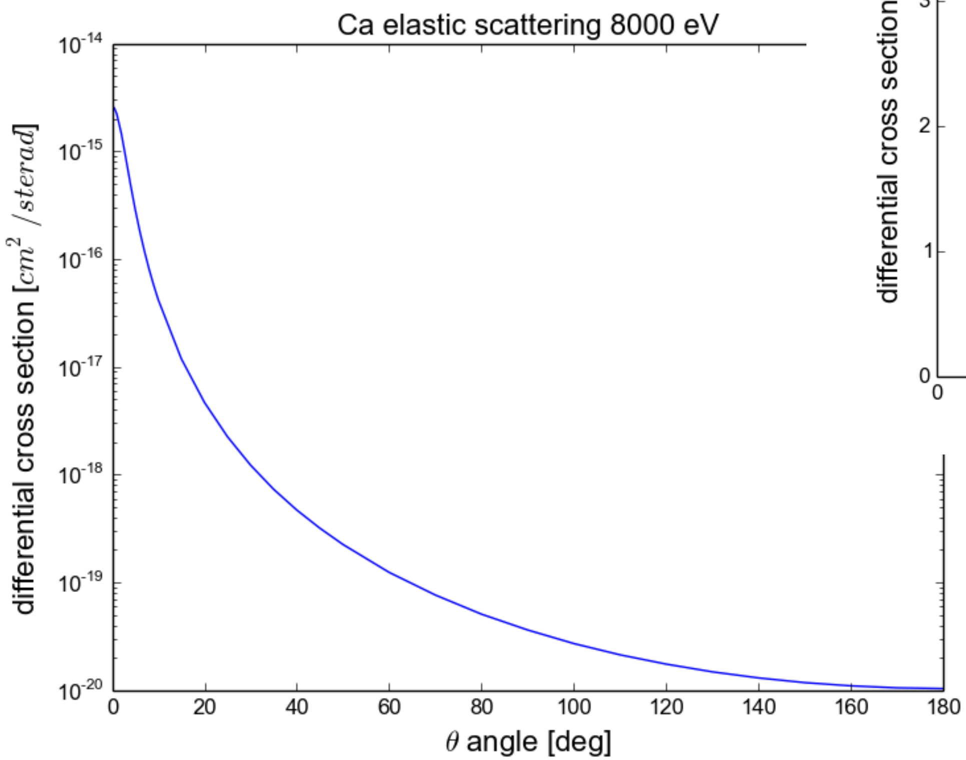


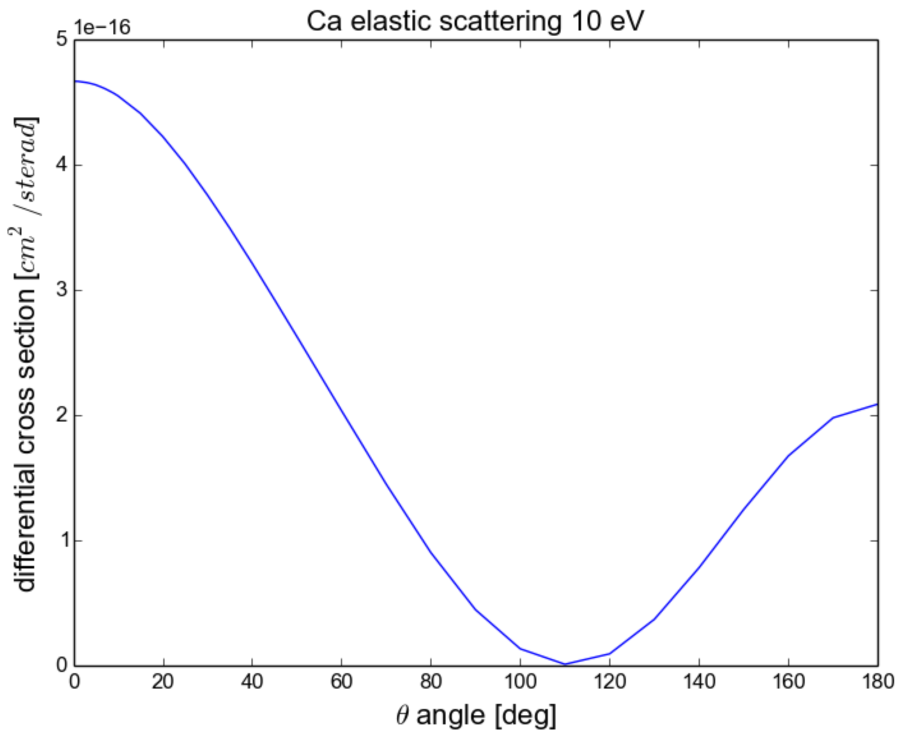
X-Rays - Differential cross section – inelastic scattering





Electrons - Differential elastic cross section





Data from: http://www.ioffe.rssi.ru/ES/Elastic/

X-ray differential elastic cross section and the form factor

$$\frac{d\sigma_{el}}{d\Omega} = \frac{d\sigma_T}{d\Omega} \left| F(x,Z) \right|^2$$

Thomson cross section

$$\frac{d\sigma_T}{d\Omega} = \frac{r_0^2}{2}(1+\cos^2\theta)$$

Atomic form factor (atomic scattering factor)

$$F(x,Z) \qquad x = \frac{sin\frac{\theta}{2}}{\lambda}$$

Variable related to the momentum transfer

$$F(x,Z) = 4\pi \int_0^\infty r^2 \rho(r,Z) \frac{\sin(4\pi x r)}{4\pi x r} dr$$

X-ray differential elastic cross section and the form factor

… but actually there is a further dependence on energy …

$$f = f^0(x,Z) + f'(E,Z) + if''(E,Z)$$

f'' photoelectric absorption

f' corrections for photoabsorption (Kramers-Kronig dispersion)
relativistic effects, nuclear scattering

Diffraction (structure factor)

$$F(h,k,l) = \sum_j f_j e^{-M_j} e^{2\pi i(hx_j + ky_j + lz_j)}$$

X-ray differential elastic cross section and the form factor

forward scattering factors (x = theta = q = 0)

$$f = f(0, Z, E) = f_1 + i f_2$$

$$f_2 \equiv f''$$

photoabsorption

$$\mu_a = 2 r_0 \lambda f_2$$

$$f_1 \equiv f^0(x = 0) + f'$$

f1 and f2 are directly related to the index of refraction (reflection, refraction, XRR)

$$n = 1 - \frac{1}{2\pi} N r_0 \lambda^2 (f_1 + i f_2)$$

$$n = 1 - \delta - i\beta$$

X-ray differential inelastic cross section (Compton)

$$\frac{d\sigma_i}{d\Omega} = \frac{d\sigma_{KN}}{d\Omega} S(q, Z)$$

$$\frac{d\sigma_{KN}}{d\Omega} = \frac{r_0^2}{2} P(\theta, E)$$

$$P(\theta, E) = \frac{1}{\left(1+\alpha(1-\cos\theta)\right)^2}\left[1+\cos^2\theta + \frac{\alpha^2(1-\cos\theta)^2}{1+\alpha(1-\cos\theta)}\right] \qquad \alpha = \frac{E}{m_0 c^2}$$

$$S(q, Z) = \int_{\varepsilon>0} \left|F_\varepsilon(q, Z)\right|^2$$

Inelastic scattering function

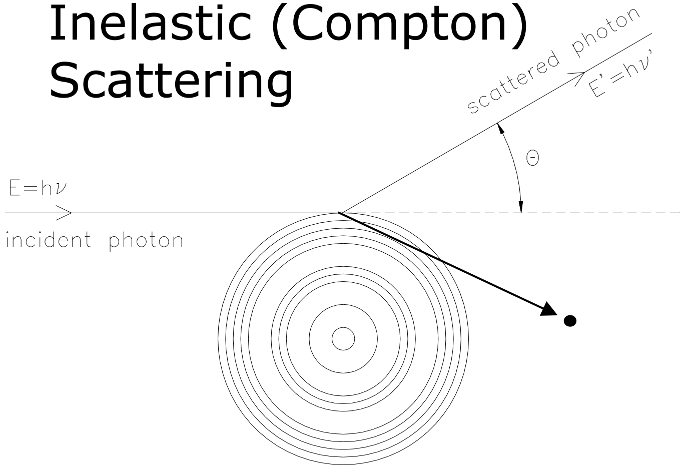
$$F_\varepsilon(\vec{q}, Z) = \sum_{n=1}^{Z} \left\langle \Psi_\varepsilon \middle| \exp(i\vec{q}\cdot\vec{r}_n) \middle| \Psi_0 \right\rangle$$

form factor elastic scattering

$$F(\vec{q}, Z) = \sum_{n=1}^{Z} \left\langle \Psi_0 \middle| \exp(i\vec{q}\cdot\vec{r}_n) \middle| \Psi_0 \right\rangle$$

X-ray inelastic (Compton) scattering

Inelastic (Compton) Scattering



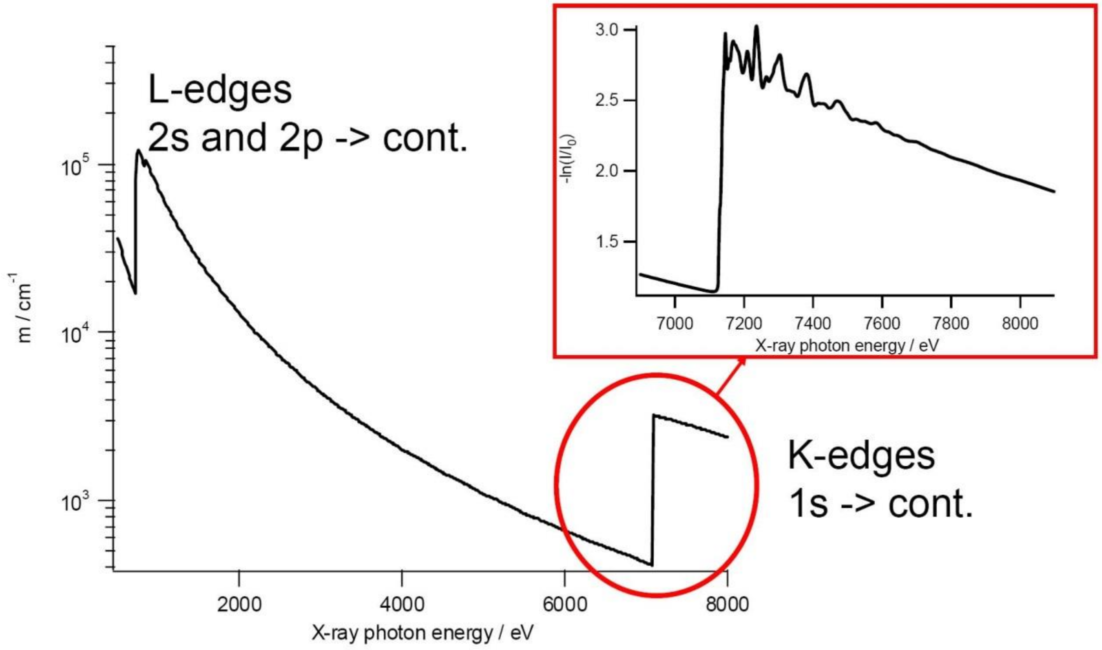
$$\lambda - \lambda' = \frac{h}{m_e c}(1 - \cos\theta)$$

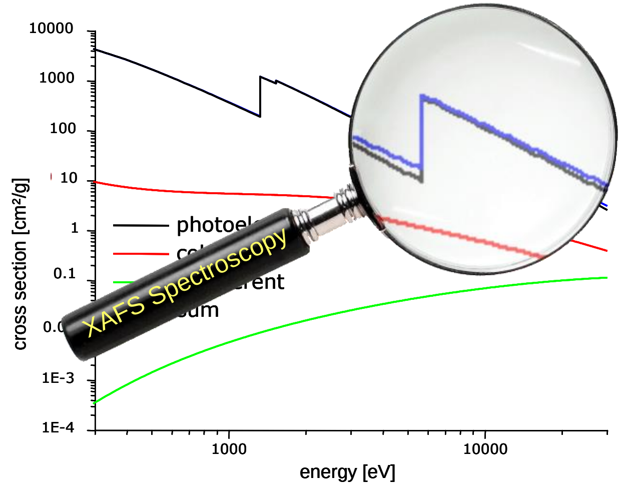
$$E' = \frac{E}{1 + \frac{E}{m_0 c^2}(1 - \cos\theta)}$$

in a spectrum the Compton peak is broader due to the angle dependence (in the accepted solid angle there are different scattering angles) and due to Doppler broadening

X-Ray Absorption near edge fine structure

The X-ray Absorption Fine Structure (XAFS) of an iron foil





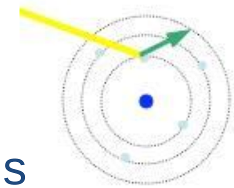
Different phenomena for:

- ‘free’ atoms
- molecules
- condensed systems

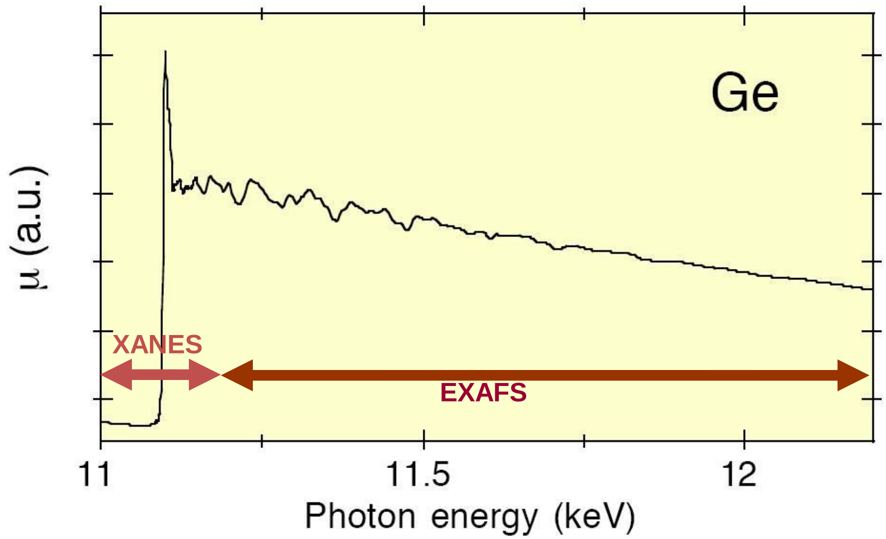
X-Ray Absorption near edge fine structure

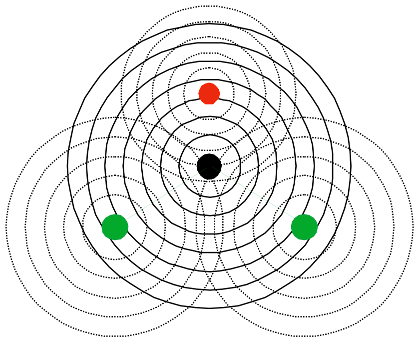
$E_{ph} \sim E_b$

Core electron → unoccupied levels



⇨ Edge fine structure (XANES or NEXAFS)





$E_{ph} > E_b$

Core electron → continuum → *outgoing wavefunction* → Backscattering from neighbouring atoms → *incoming wavefunction*

INTERFERENCE (between outgoing and incoming wavefunction) → Extended fine structure (EXAFS)

FONDAZIONE
BRUNO KESSLER

Thank you for your attention!