Radiation interaction with matter and energy dispersive x-ray fluorescence analysis (EDXRF)

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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

$$E_k = eV = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

$$\lambda = \frac{h}{\sqrt{2meV}} \frac{1}{\sqrt{1 + \frac{eV}{2mc^2}}}$$

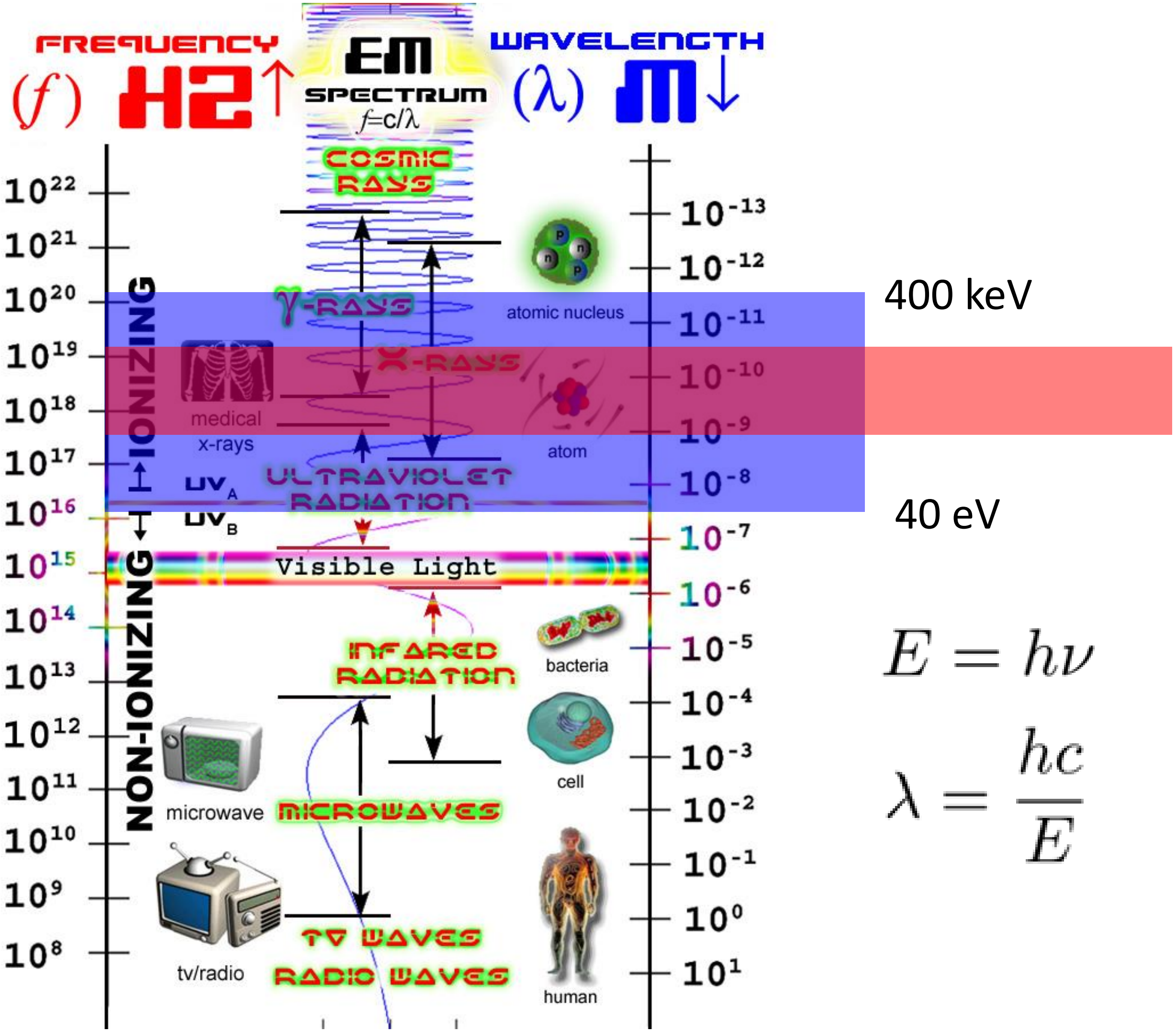
Radiation – x-rays (photons) , neutrons, electrons

	interaction type	interaction partners
x-rays **photons**	dipole	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 – x-rays (photons) , neutrons, electrons



400 keV

40 keV

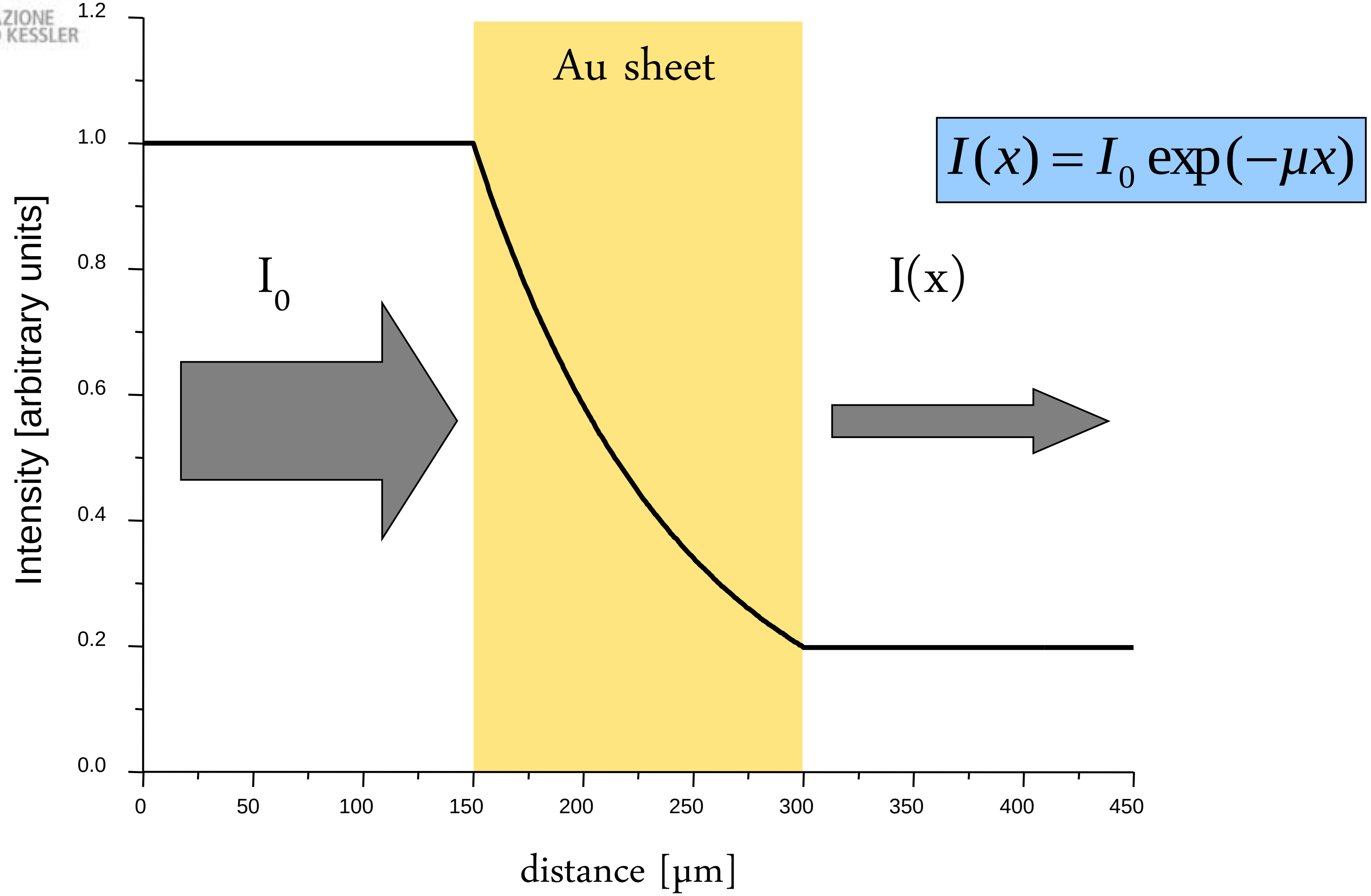
1 keV

40 eV

$$E = h\nu$$

$$\lambda = \frac{hc}{E}$$

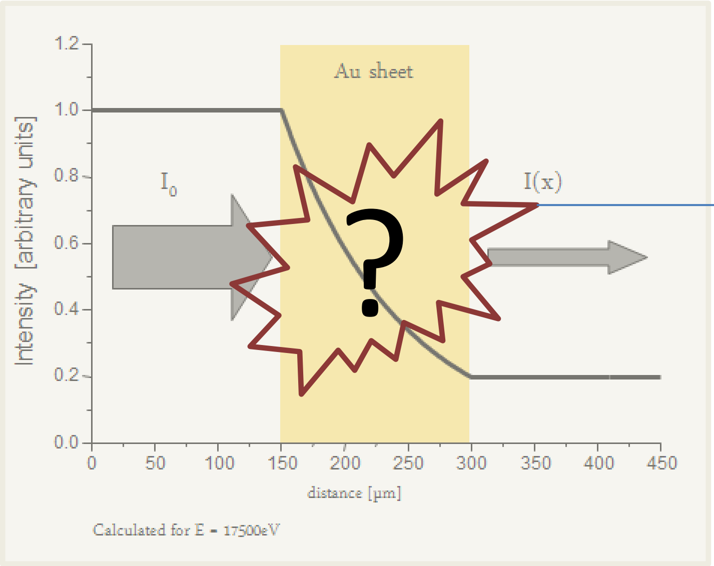
Radiation – attenuation - Beer Lambert law



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

Calculated for X-Rays E = 17500eV

Radiation – attenuation - Beer Lambert law



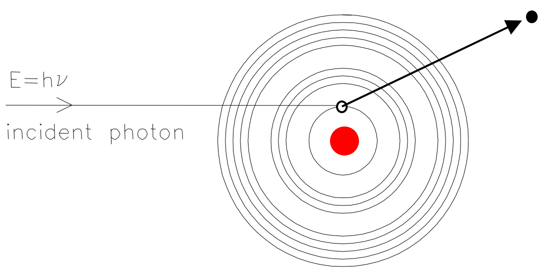
Scattering
(elastic, inelastic)
Absorption

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

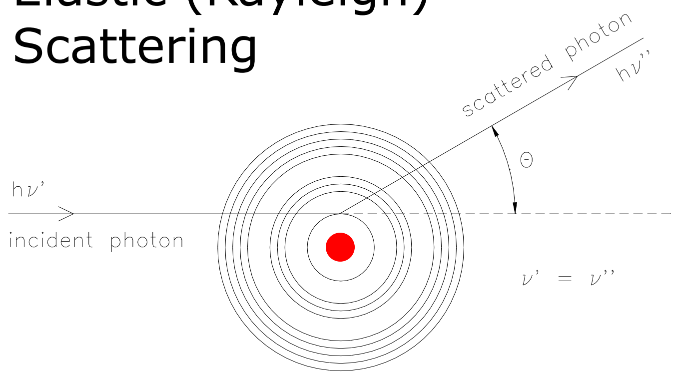
$$\mu = \mu_a + \mu_s$$

Attenuation X-Rays : microscopic view

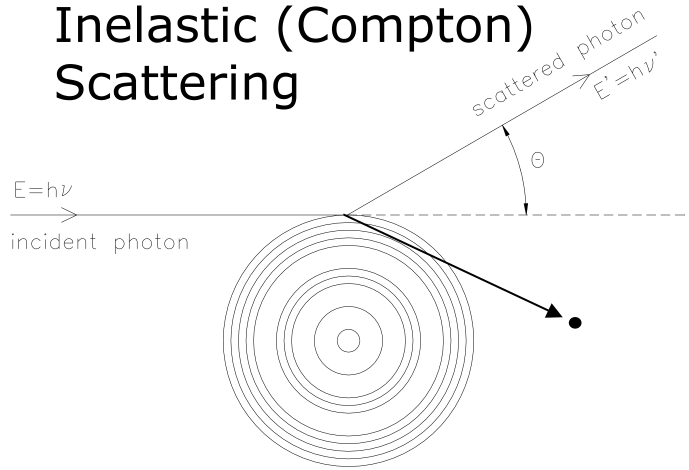
Photoelectric absorption



Elastic (Rayleigh) Scattering



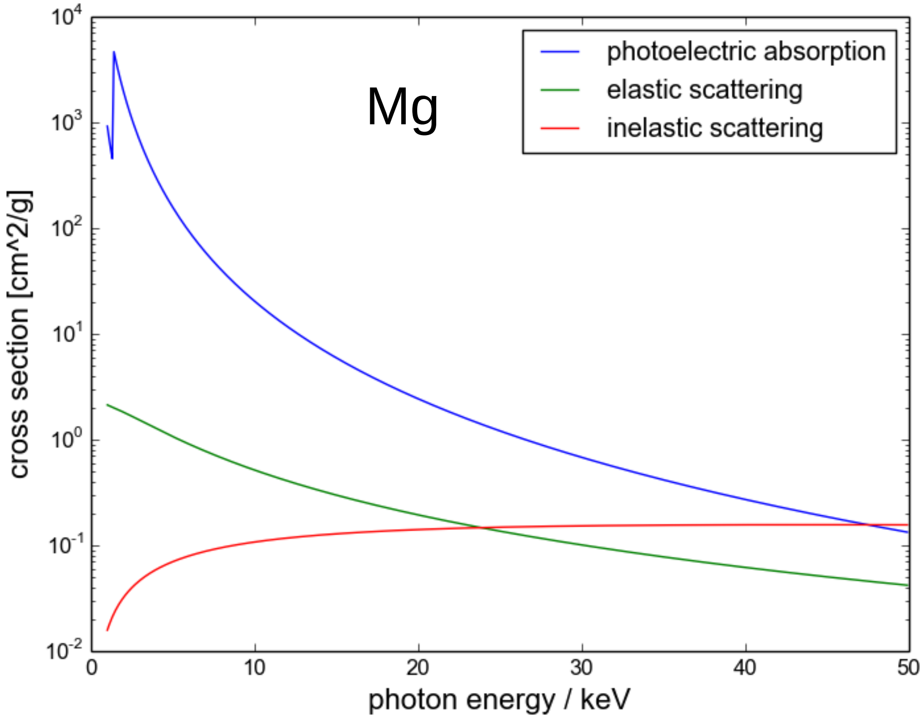
Inelastic (Compton) Scattering

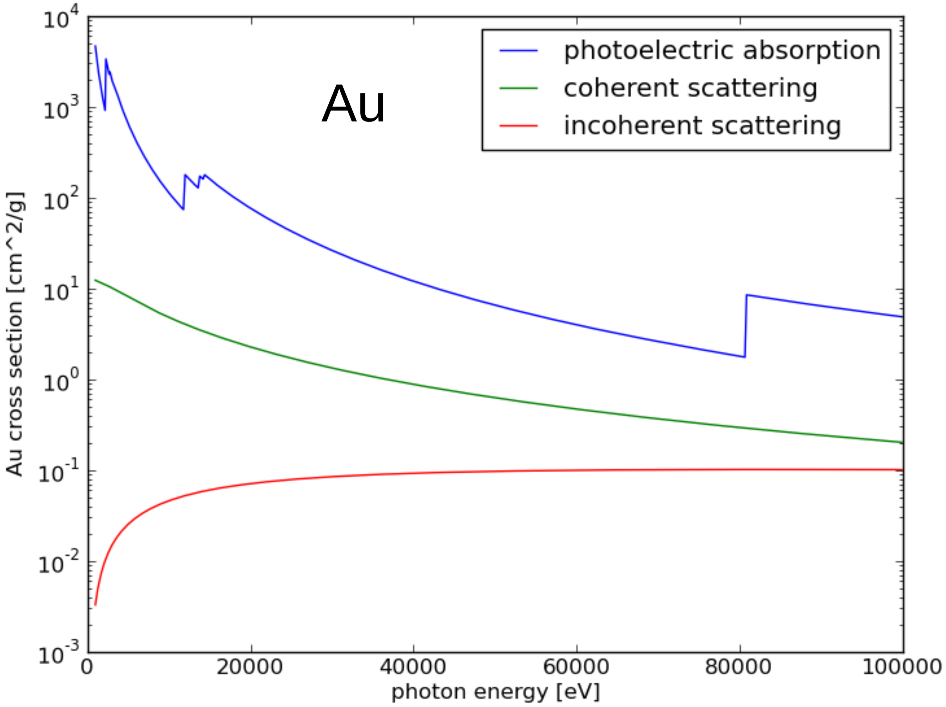


X-Rays cross section magnitude

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

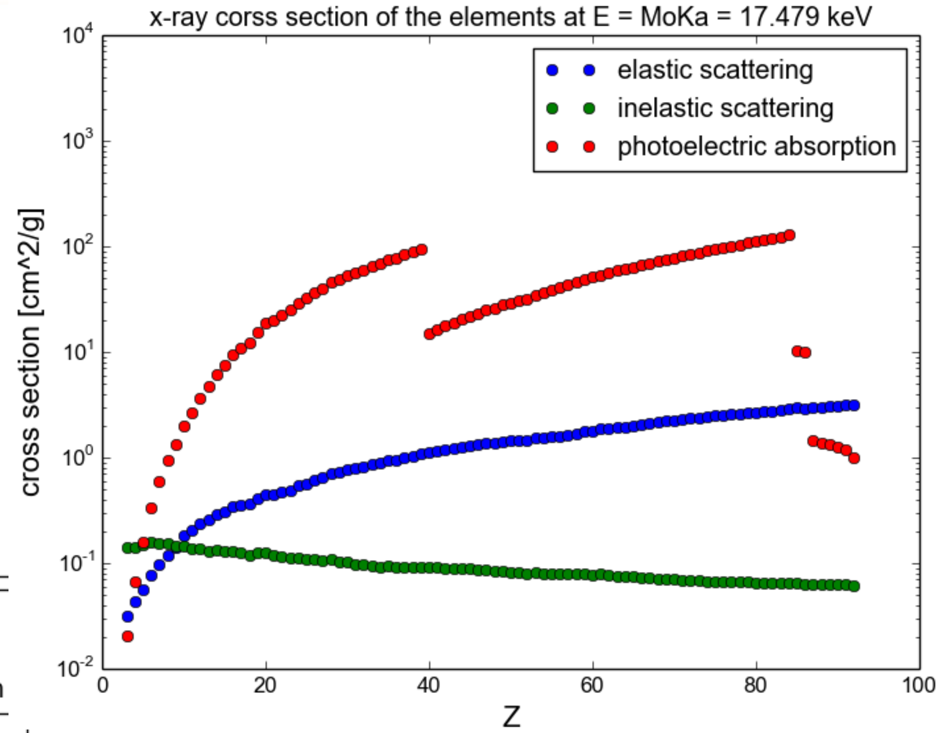
$$\mu = \sigma_c + \sigma_i + \tau$$

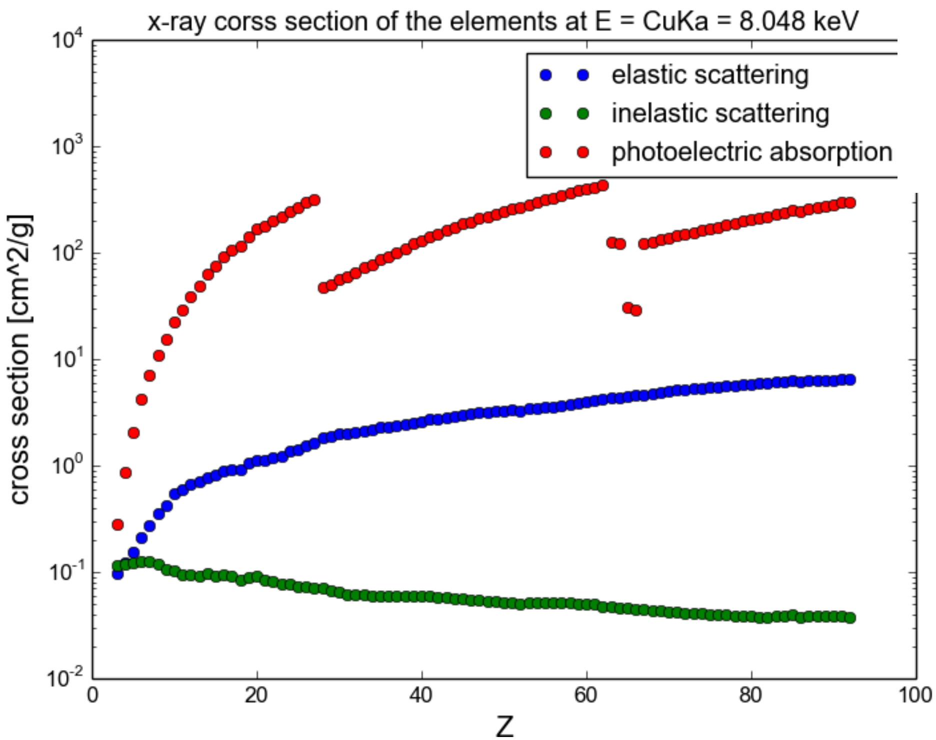




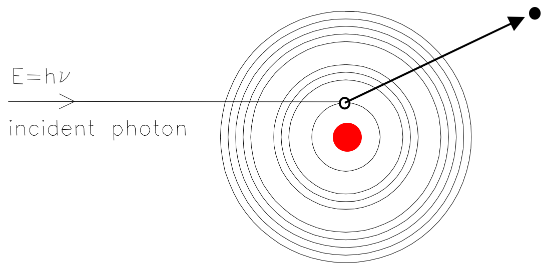
data from:
H. Ebel, R. Svagera, M. F. Ebel, A. Shaltout and J. H. Hubbell,
Numerical description of photoelectric absorption coefficients for fundamental parameter programs,
X-Ray Spectrometry, 32, 442–451 (2003)

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

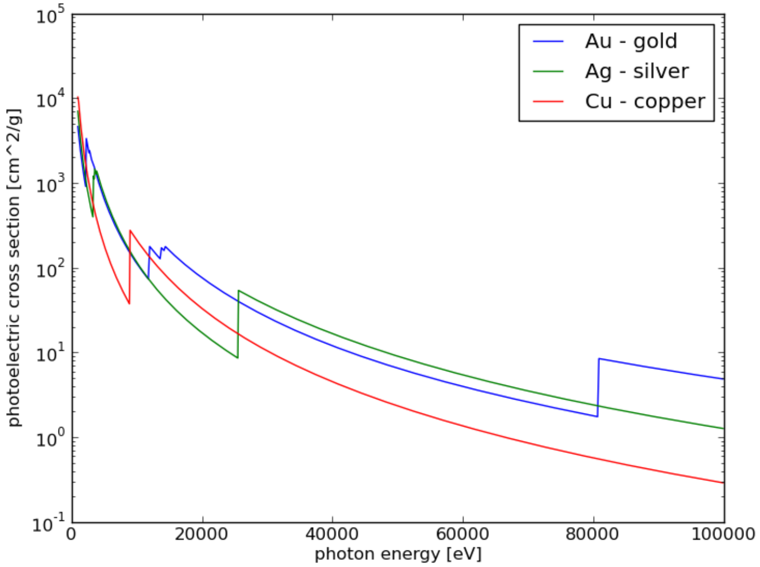


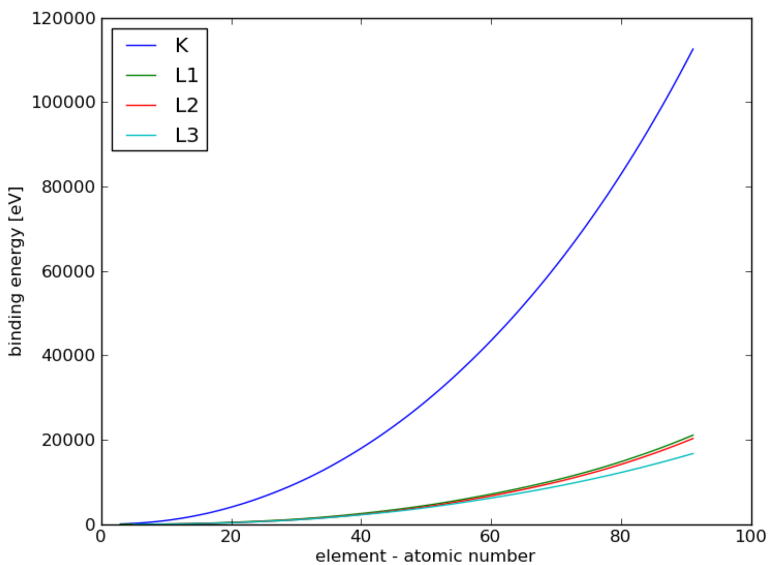
Absorption edges
Electron energy levels
Shells

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

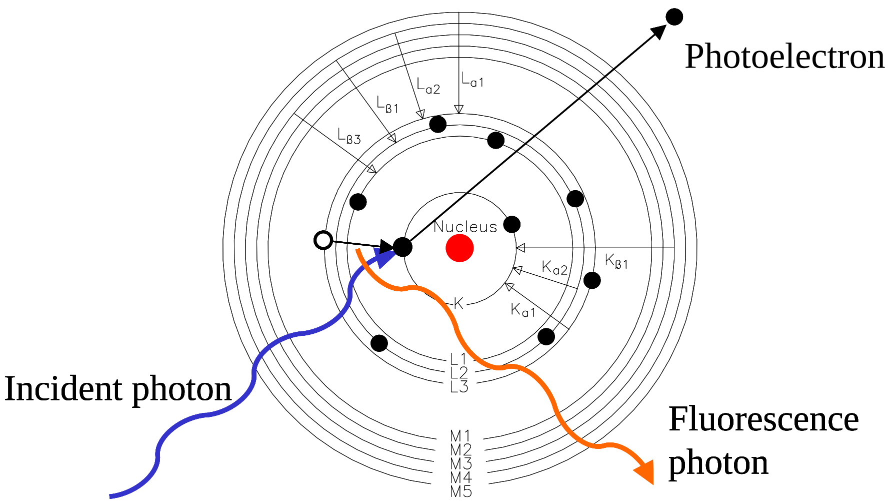
Z	shell	energy_eV	jump	level_width_eV
79	K	80724.9	4.874	52.1
79	L1	14352.8	1.15567	9.8
79	L2	13733.6	1.4	5.53
79	L3	11918.7	2.55	5.54
79	M1	3424.9	1.04	15.0
79	M2	3147.8	1.058	9.5
79	M3	2743.0	1.15776	8.5
79	M4	2291.1	1.07	2.18
79	M5	2205.7	1.092	2.18

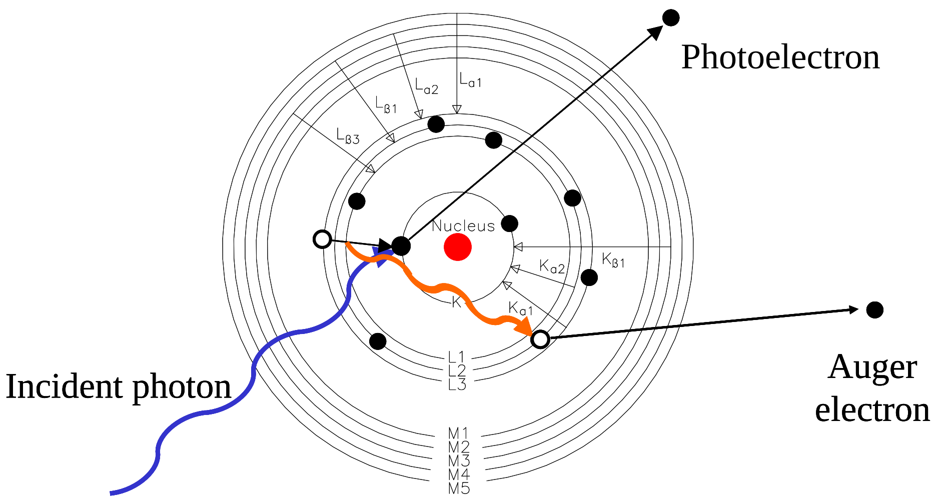
www.txrf.org/xraydata

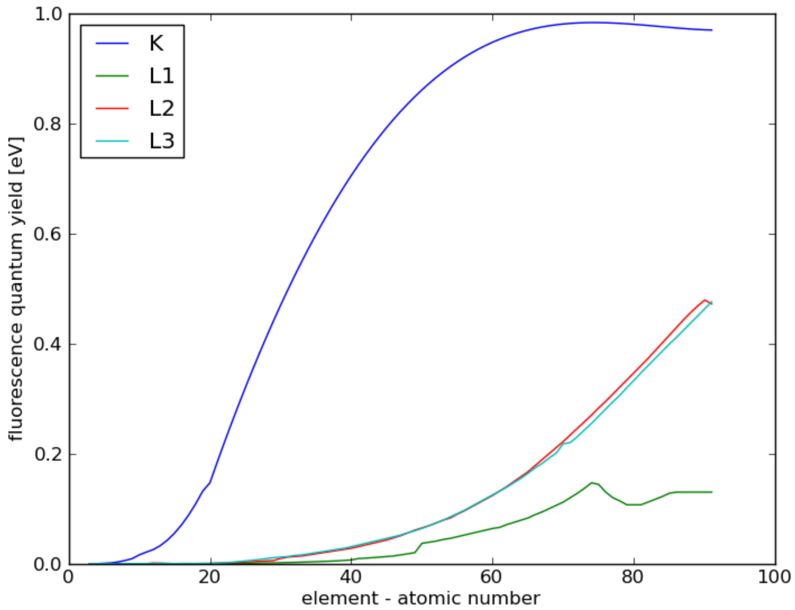




Secondary effects – fluorescence vs Auger





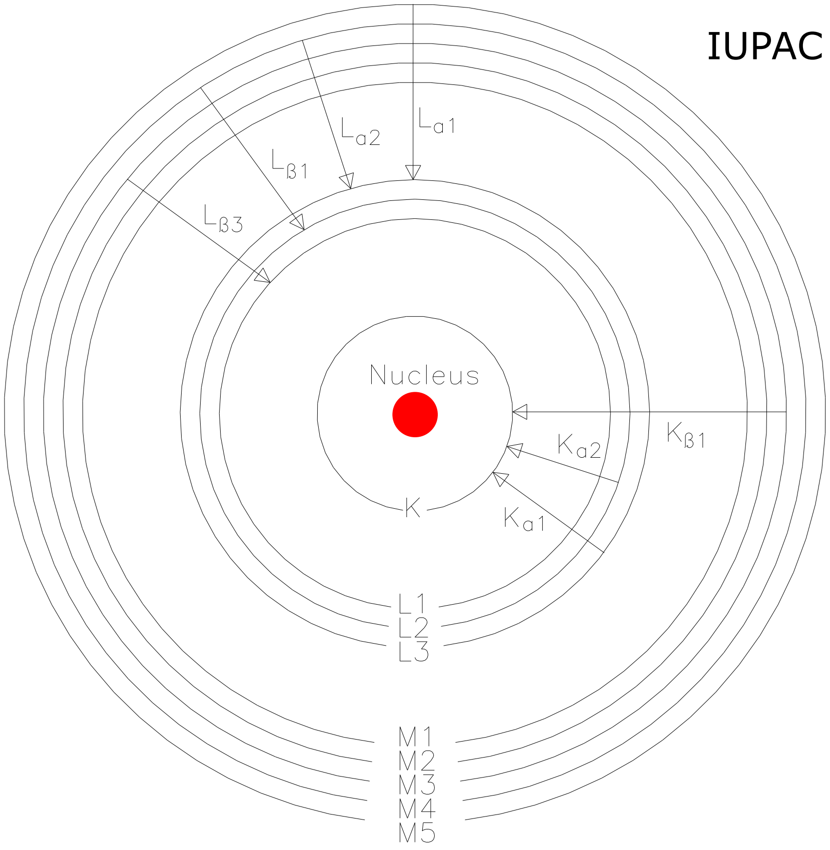


data from:
M. O. Krause,
J. Phys. Chem. Ref. Data 8 (1979) 307

X-Ray Fluorescence – characteristic lines

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

IUPAC = International Union of Pure and Applied Chemistry

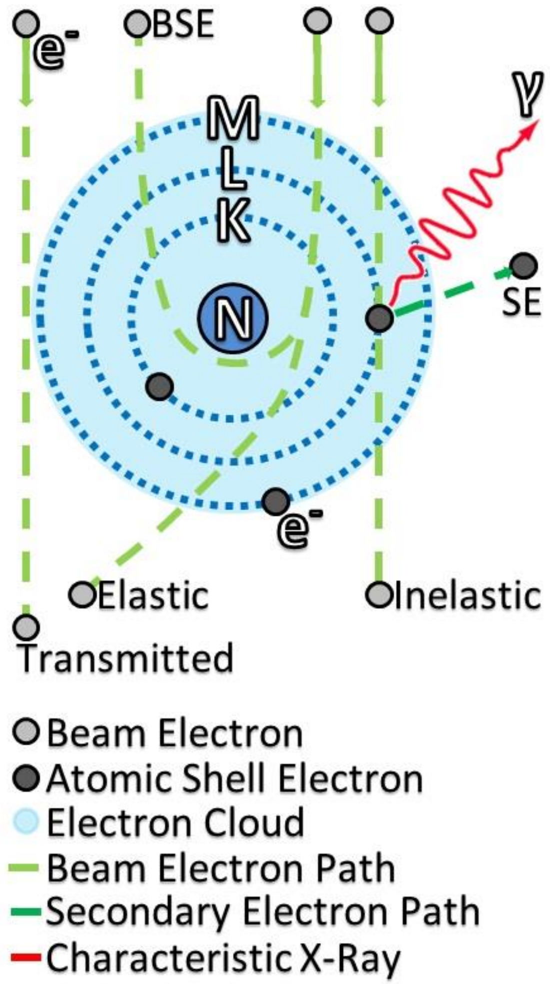


Siegbahn	IUPAC	Siegbahn	IUPAC
$K\alpha_1$	K-L3	$L\alpha_1$	L3-M5
$K\alpha_2$	K-L2	$L\alpha_2$	L3-M4
$K\beta_1$	K-M3	$L\beta_1$	L2-M4
$K\beta_2$	K-N2,N3	$L\beta_2$	L3-N5
$K\beta_3$	K-M2	$L\beta_3$	L1-M3
		$L\beta_4$	L1-M2

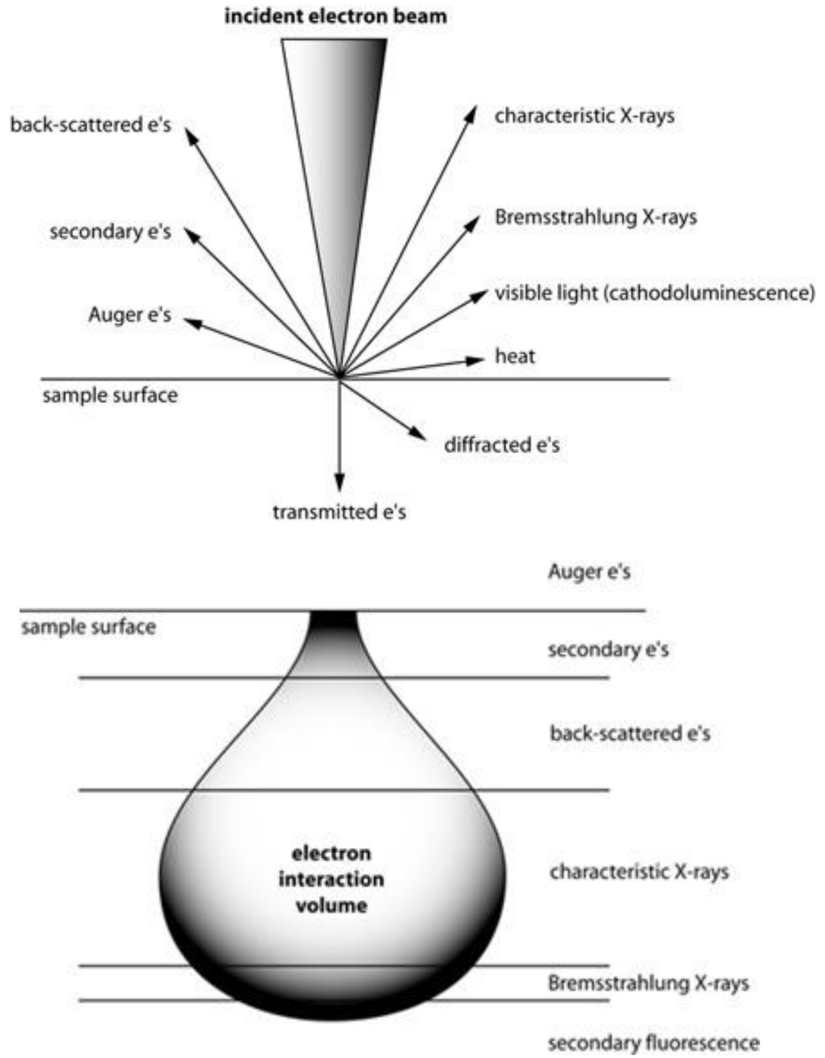
Germanium

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

Electrons interaction with matter

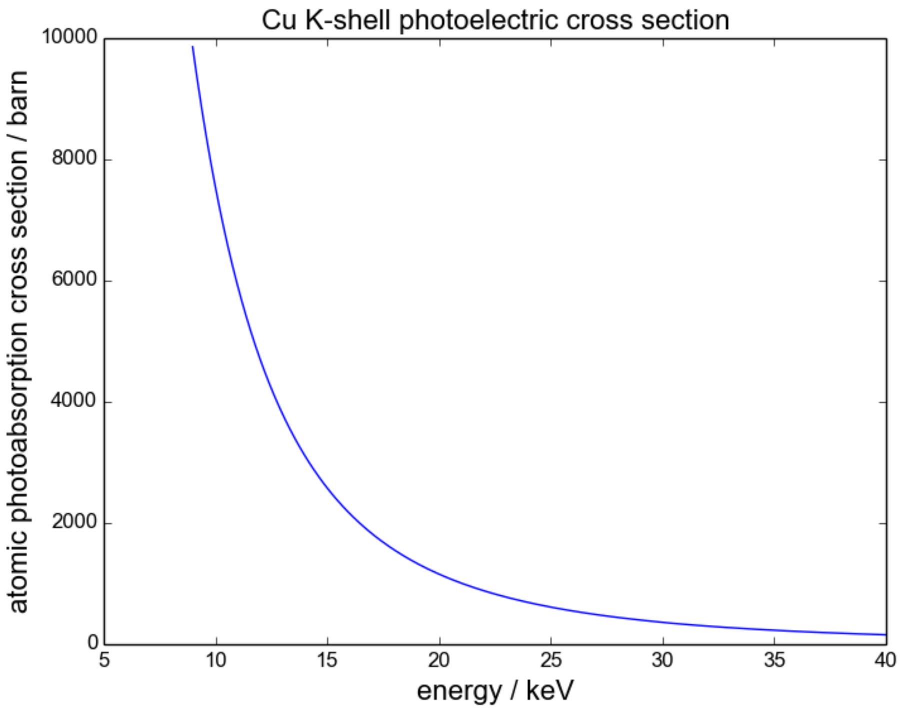


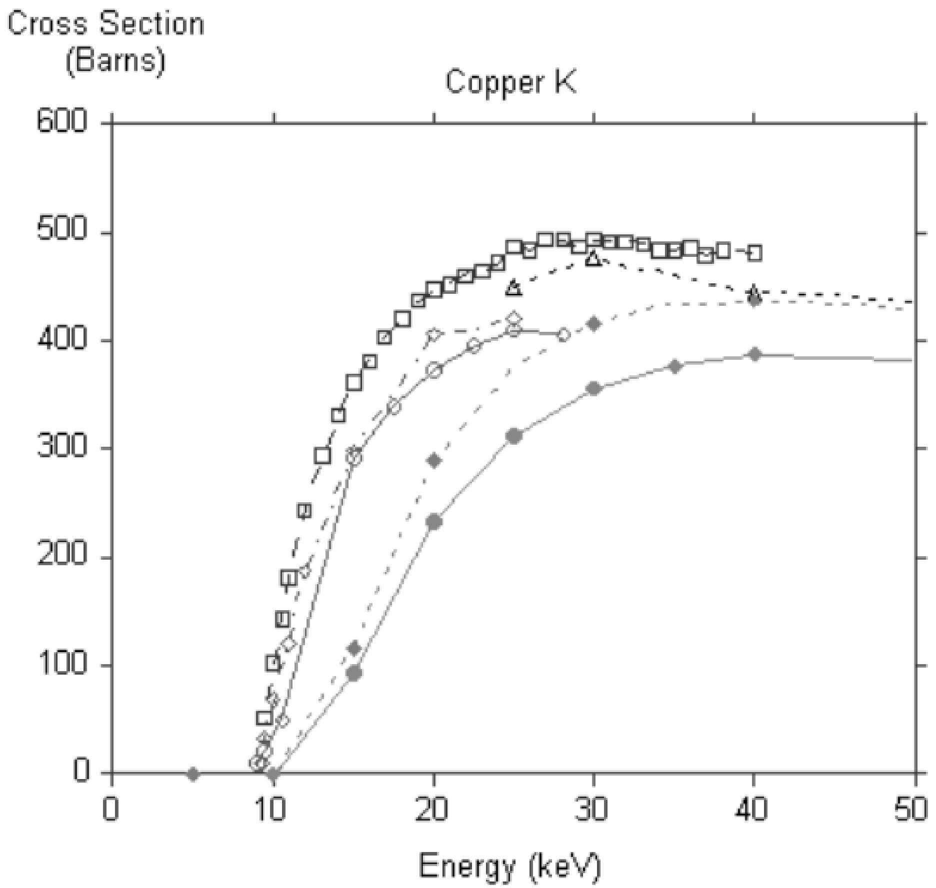
https://en.wikipedia.org/wiki/Electron_scattering

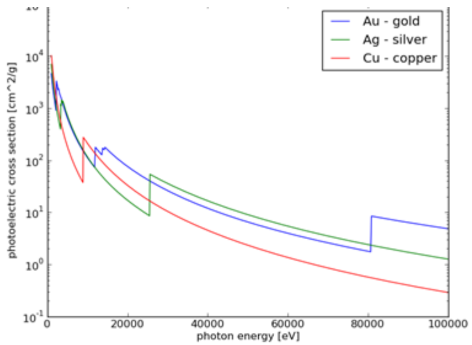


http://serc.carleton.edu/research_education/geochemsheets/electroninteractions.html

Inner shell ionization cross section: x-rays vs electrons







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Neutrons interaction with matter

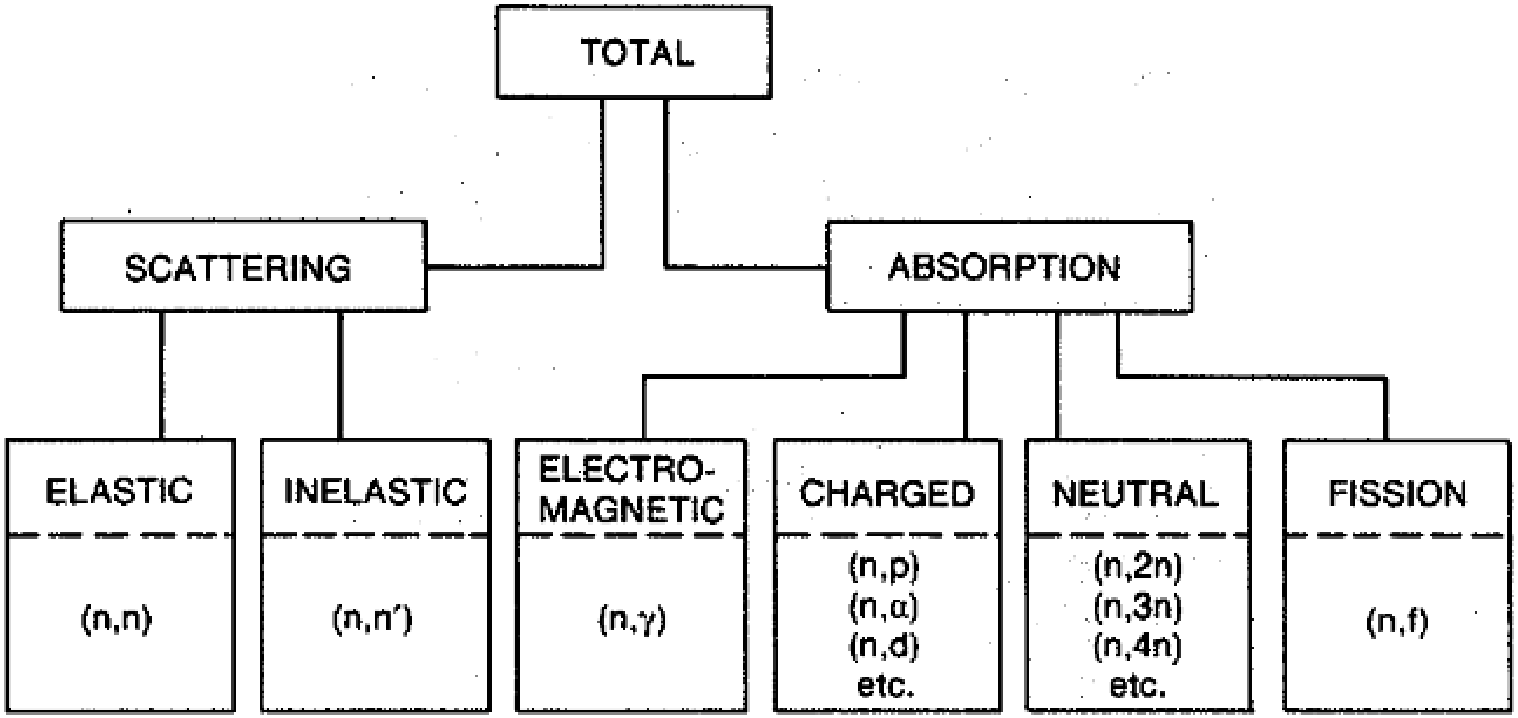
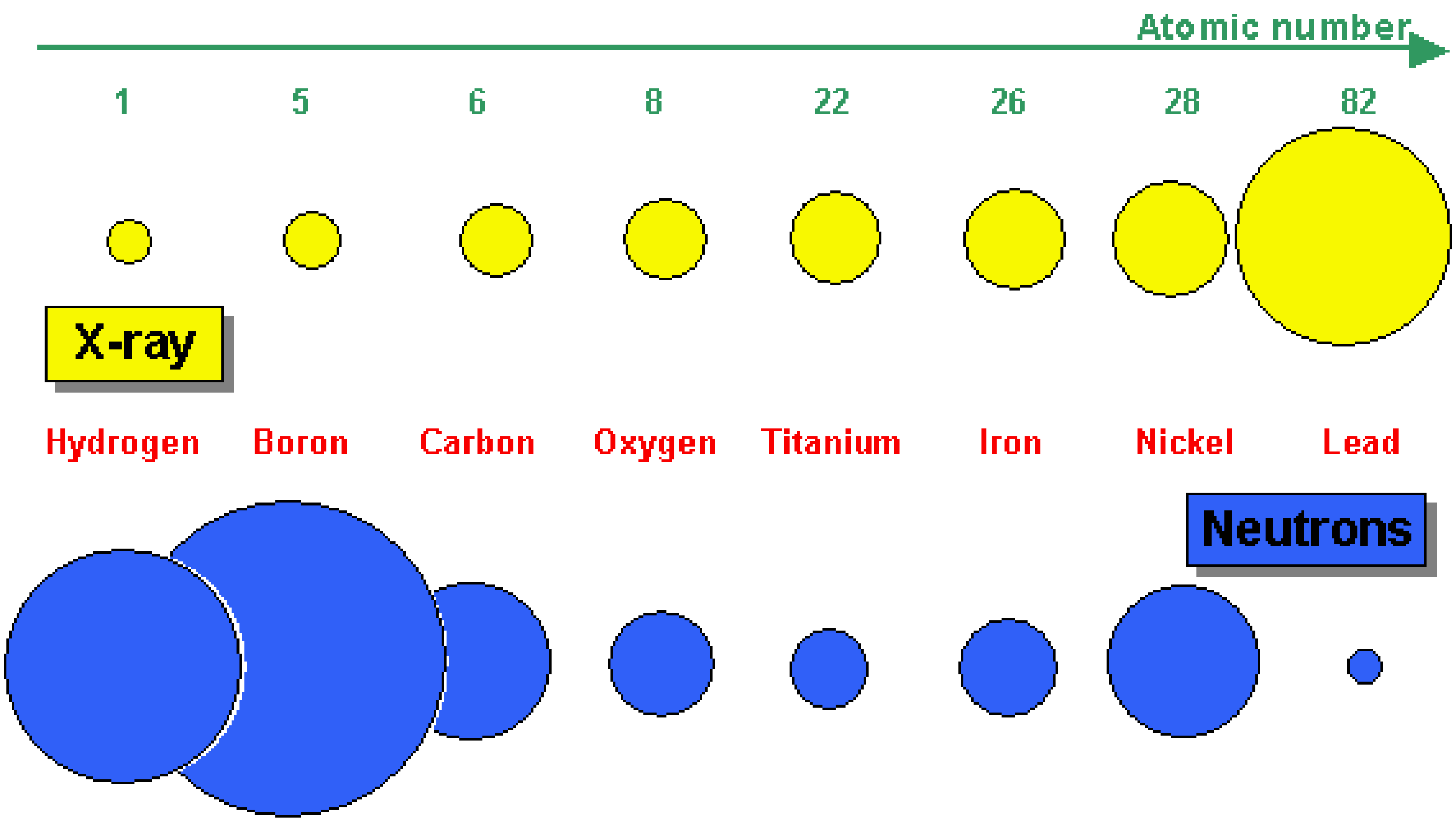


Fig. 12.2 *Various categories of neutron interactions. The letters separated by commas in the parentheses show the incoming and outgoing particles.*

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]

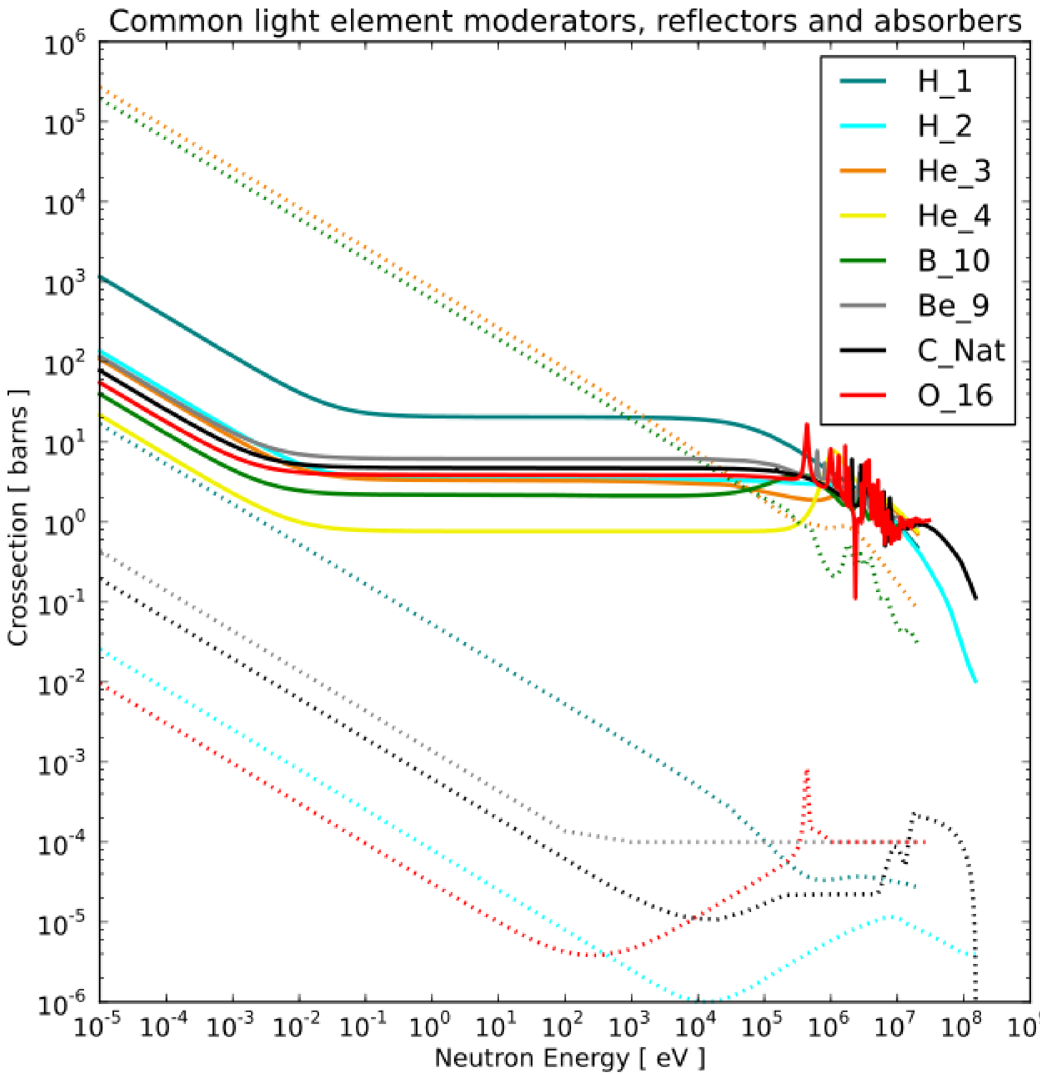
	1a	2a	3b	4b	5b	6b	7b	8			1b	2b	3a	4a	5a	6a	7a	0
	H 3.44																	He 0.02
	Li 3.30	Be 0.79											B 101.60	C 0.56	N 0.43	O 0.17	F 0.20	Ne 0.10
	Na 0.09	Mg 0.15											Al 0.10	Si 0.11	P 0.12	S 0.06	Cl 1.33	Ar 0.03
	K 0.06	Ca 0.08	Sc 2.00	Ti 0.60	V 0.72	Cr 0.54	Mn 1.21	Fe 1.19	Co 3.92	Ni 2.05	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

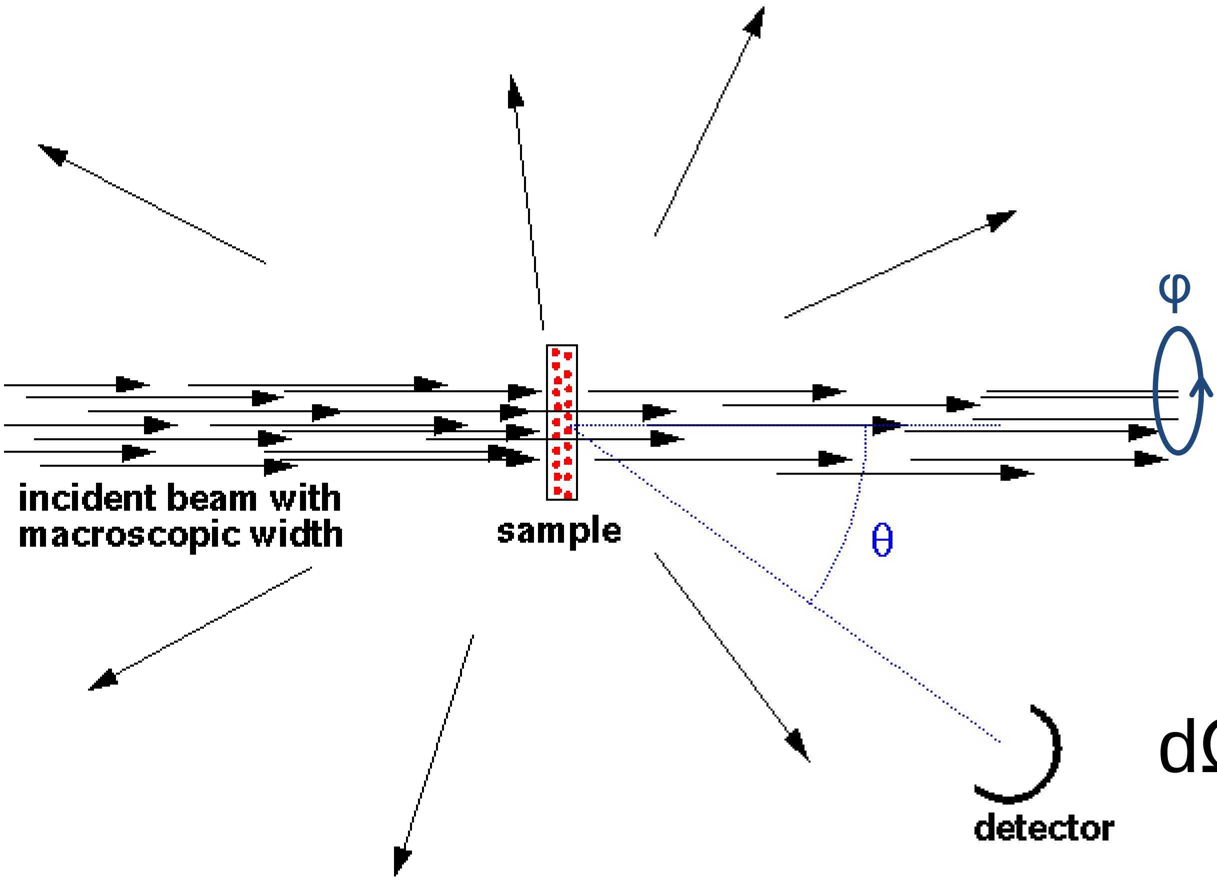


Scattering (full line) and absorption (dotted) cross sections of light element commonly used as neutron moderators, reflectors and absorbers, the data was obtained from database NEA N ENDF/B-VII.1 using JANIS software

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

Scattering - Differential cross section

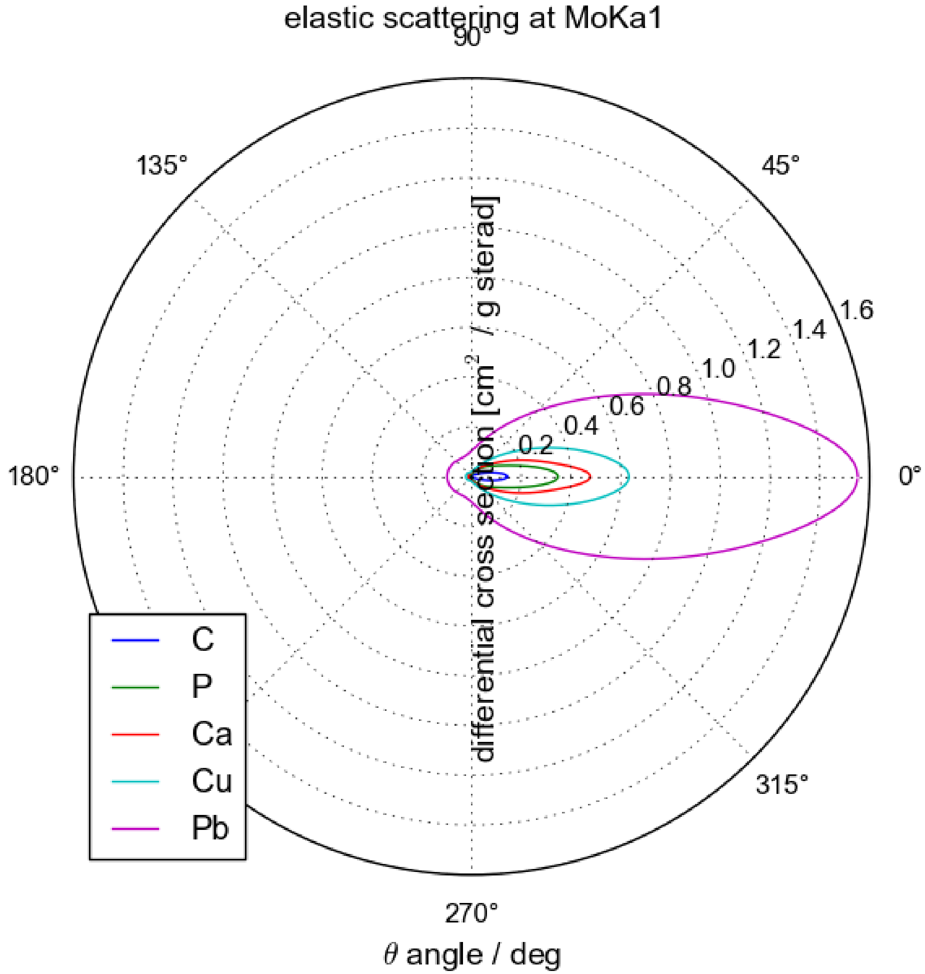
$$\frac{d\sigma}{d\Omega}$$

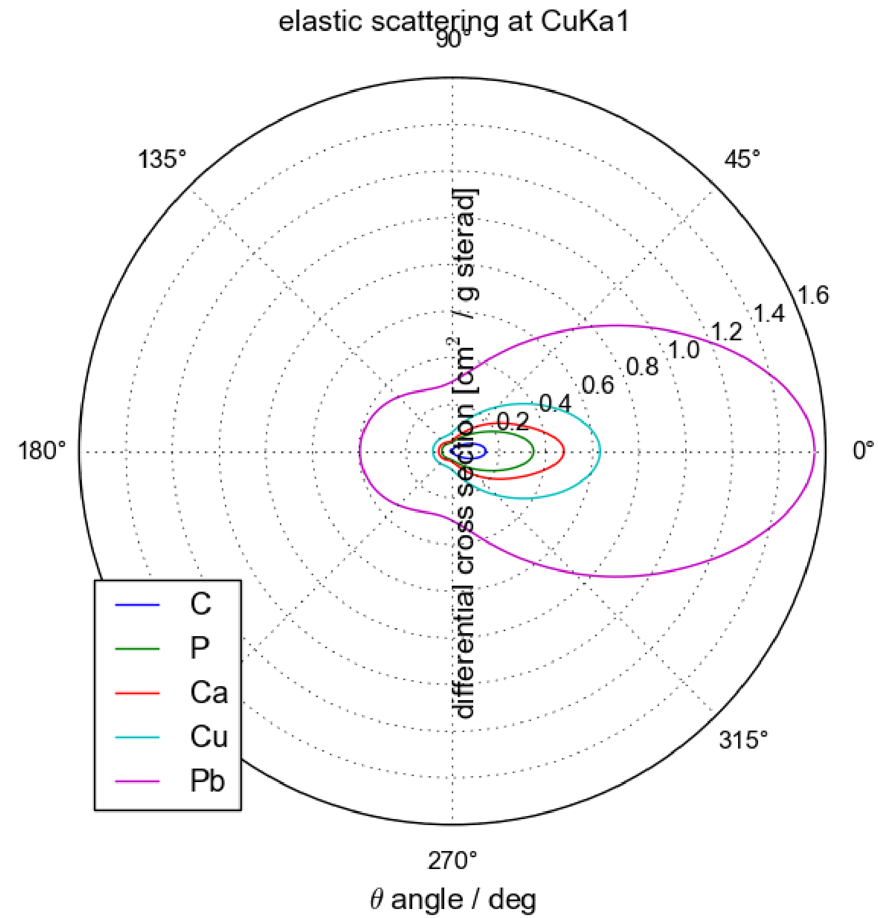


$$d\Omega = d\theta d\varphi$$

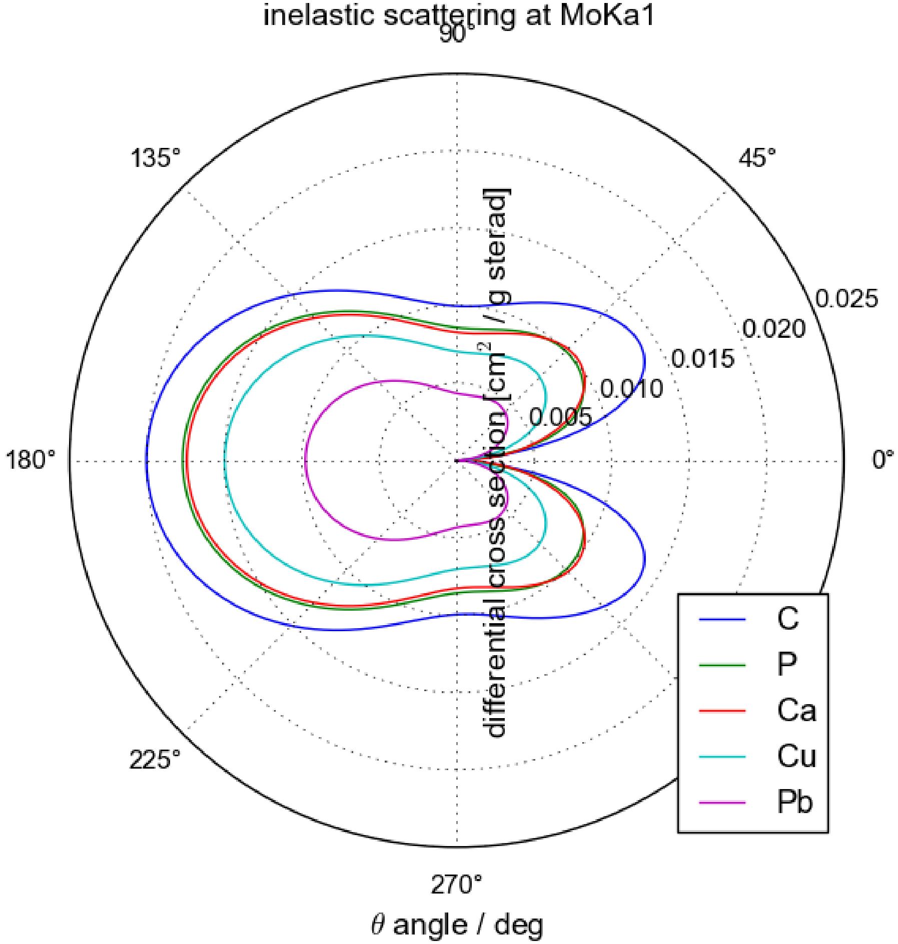
http://www.physics.csbsju.edu/QM/square.17.html

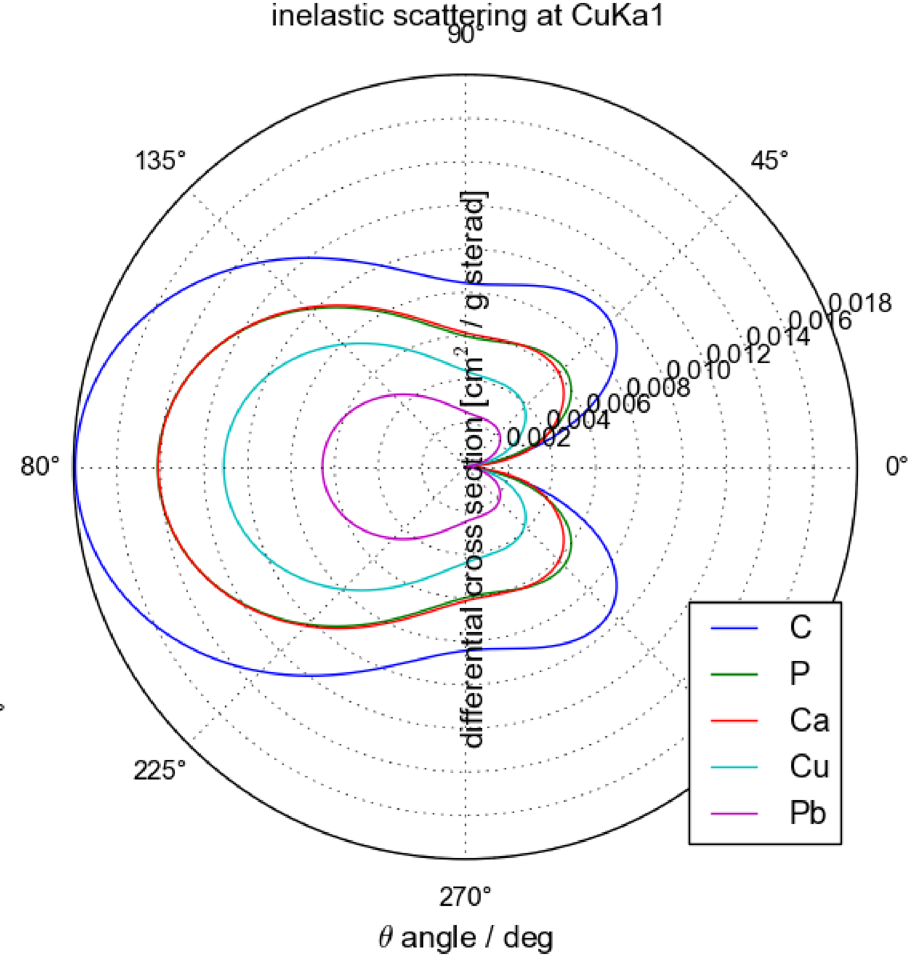
X-Rays - Differential cross section – elastic scattering



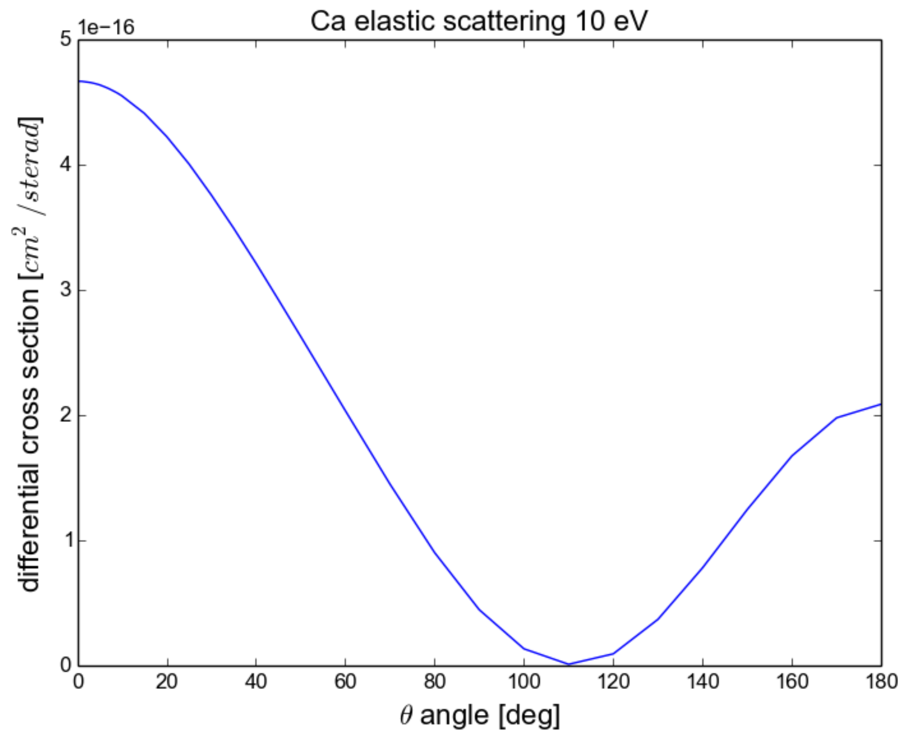


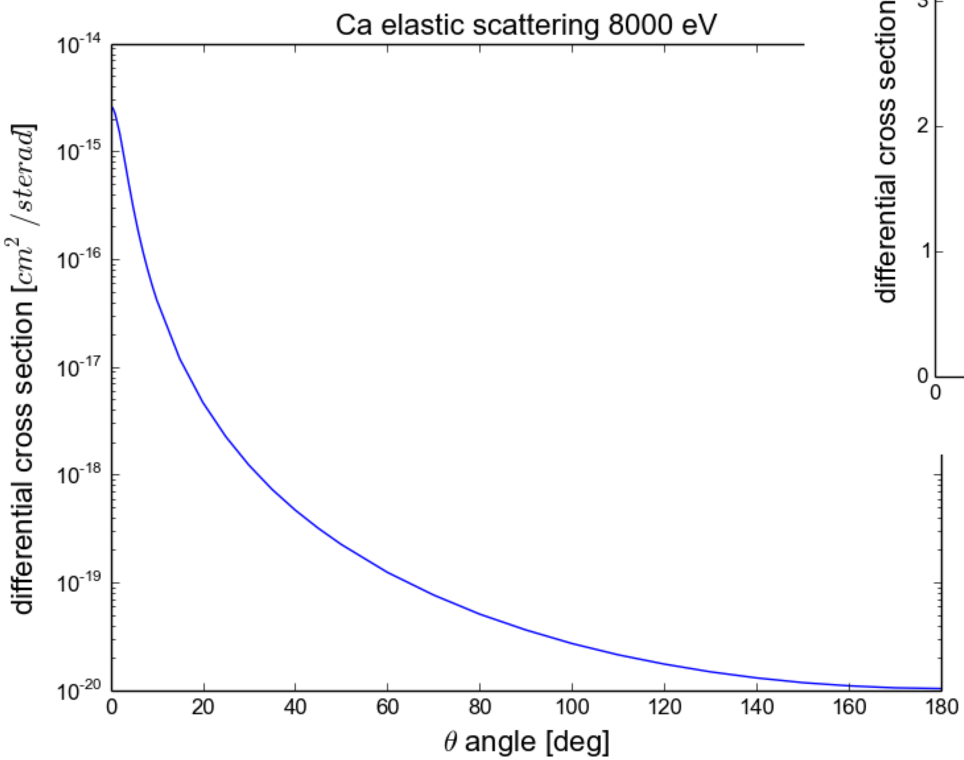
X-Rays - Differential cross section – inelastic scattering





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 …

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

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

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)

$$f = f(0, Z, E) = f_1 + if_2$$

$$f_2 \equiv f''$$

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

photoabsorption

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

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

$$n = 1 - \frac{1}{2\pi}Nr_0\lambda^2(f_1 + if_2)$$

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

$$\delta = \frac{1}{2\pi}Nr_0\lambda^2 f_1$$

$$\beta = \frac{1}{2\pi}Nr_0\lambda^2 f_2$$

X-ray differential inelastic cross section (Compton)

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

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

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

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

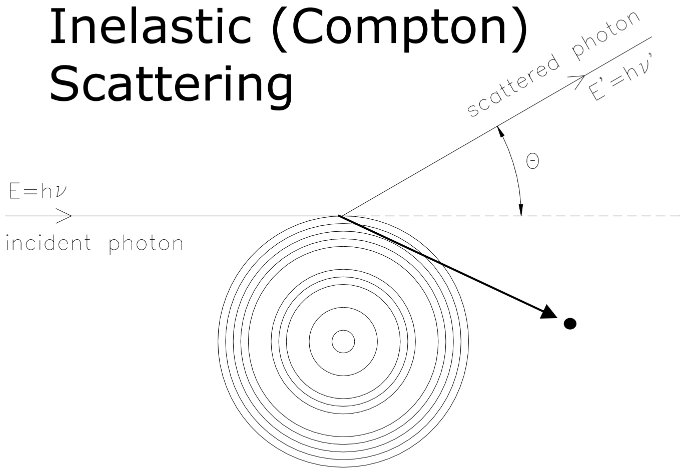
Inelastic scattering function

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

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



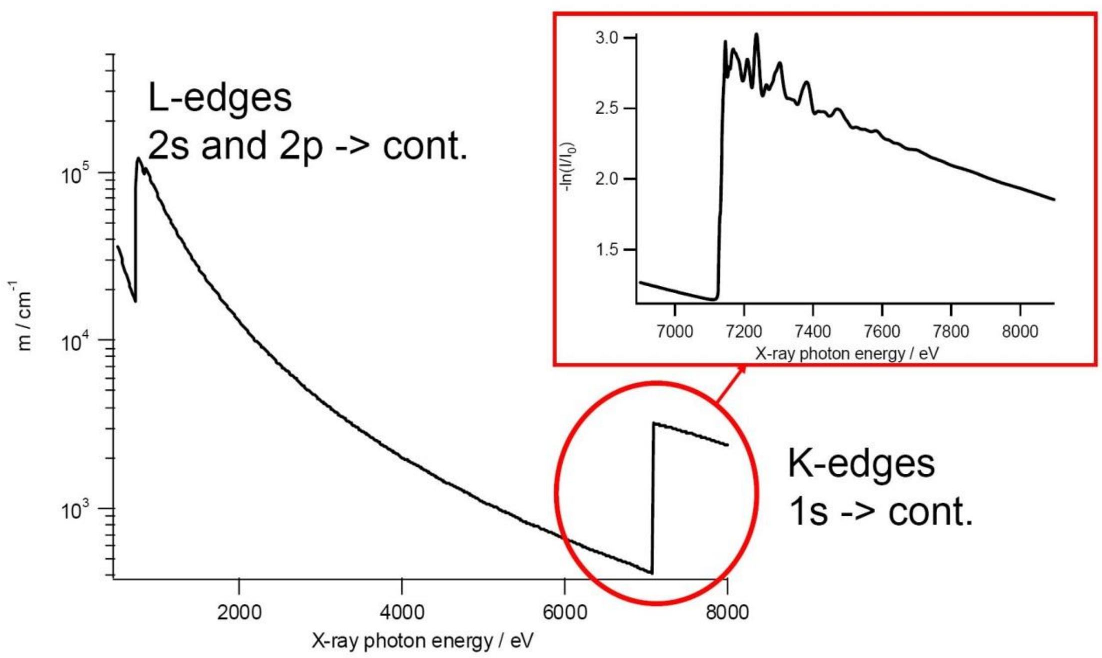
$$\lambda - \lambda' = \frac{h}{m_e c}(1 - \cos\theta)$$

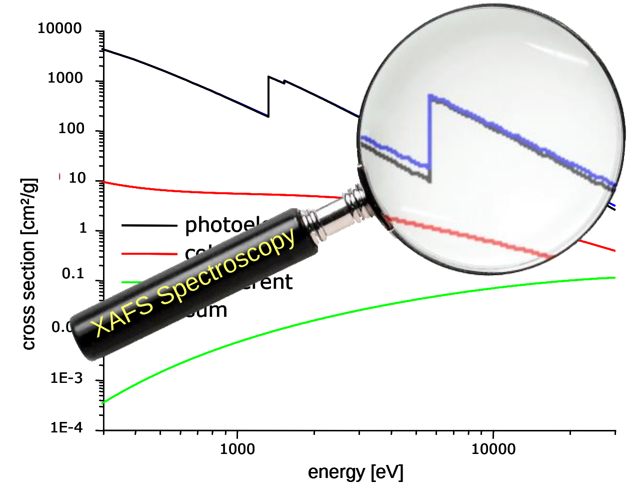
$$E' = \frac{E}{1 + \frac{E}{m_0 c^2}(1 - \cos\theta)}$$

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





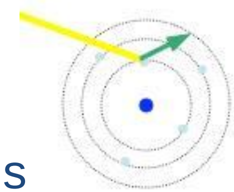
Different phenomena for:

- 'free' atoms
- molecules
- condensed systems

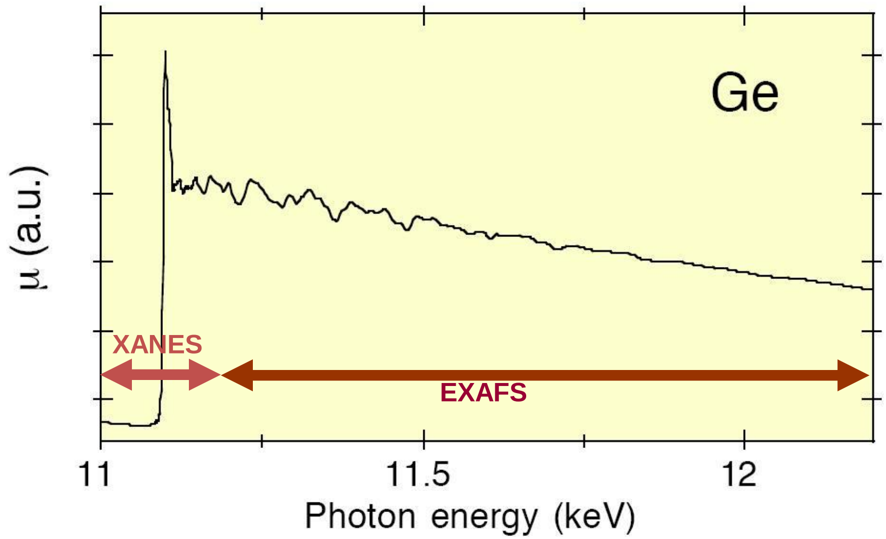
X-Ray Absorption near edge fine structure

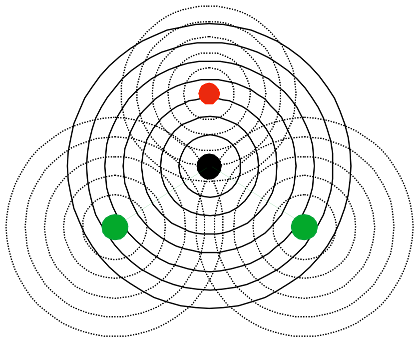
$E_{ph} \sim E_b$

Core electron → unoccupied levels



⇨ Edge fine structure (XANES or NEXAFS)





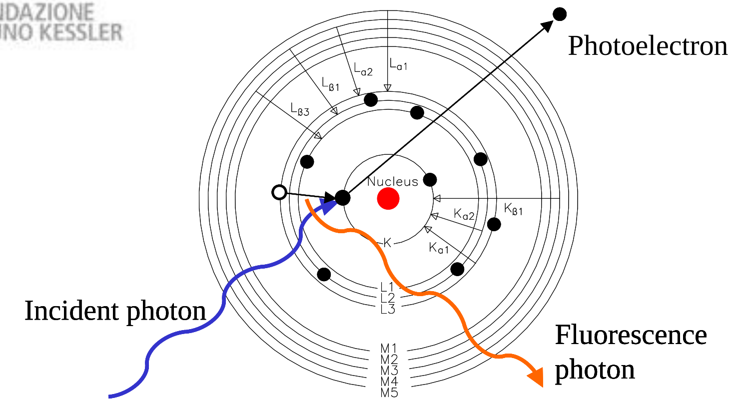
$E_{ph} > E_b$

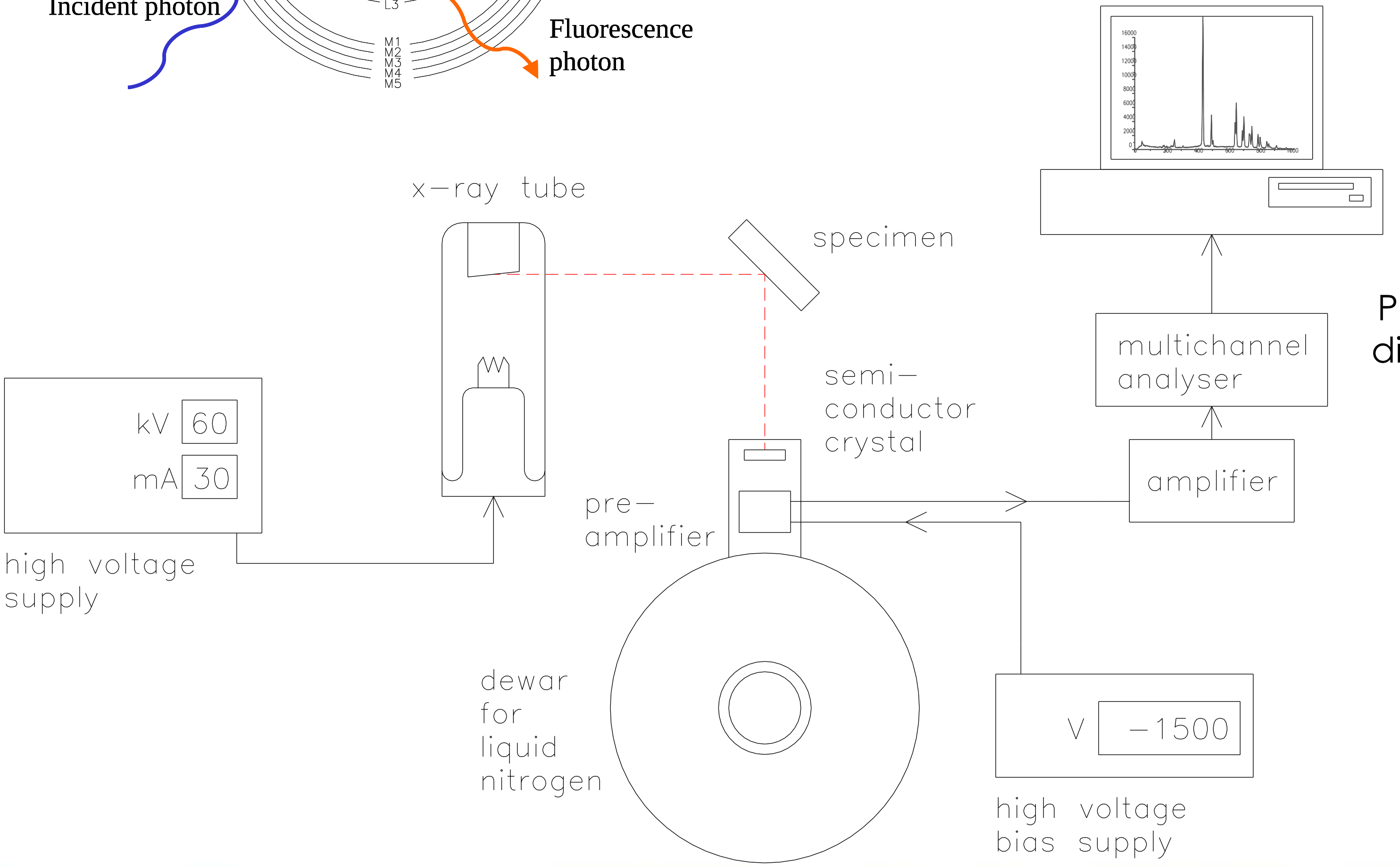
Core electron → continuum → *outgoing wavefunction* → Backscattering from neighbouring atoms → *incoming wavefunction*

INTERFERENCE ↕

Extended fine structure (EXAFS) ← INTERFERENCE

Energy Dispersive X-Ray Fluorescence analysis (EDXRF)

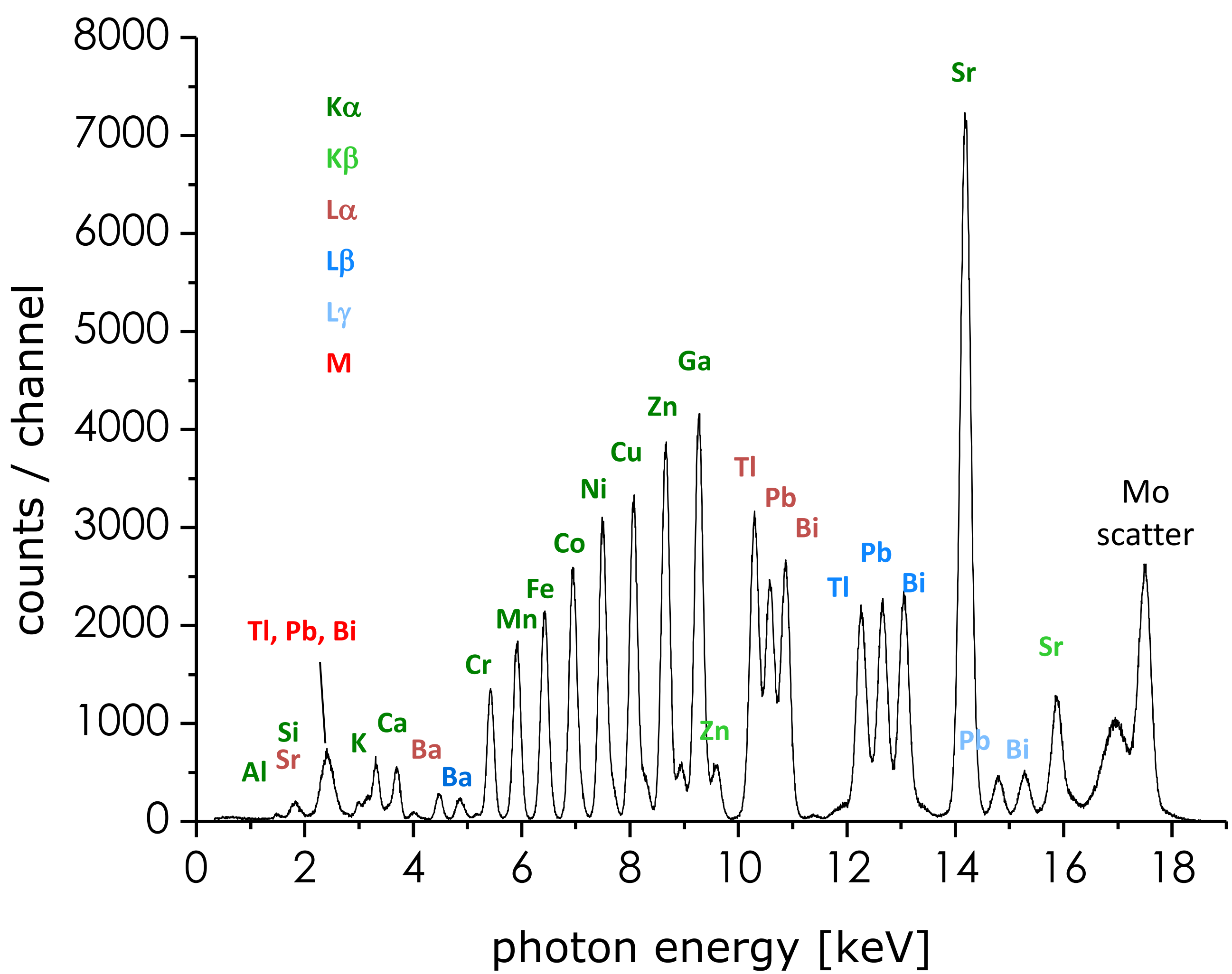




Pulse height discriminator

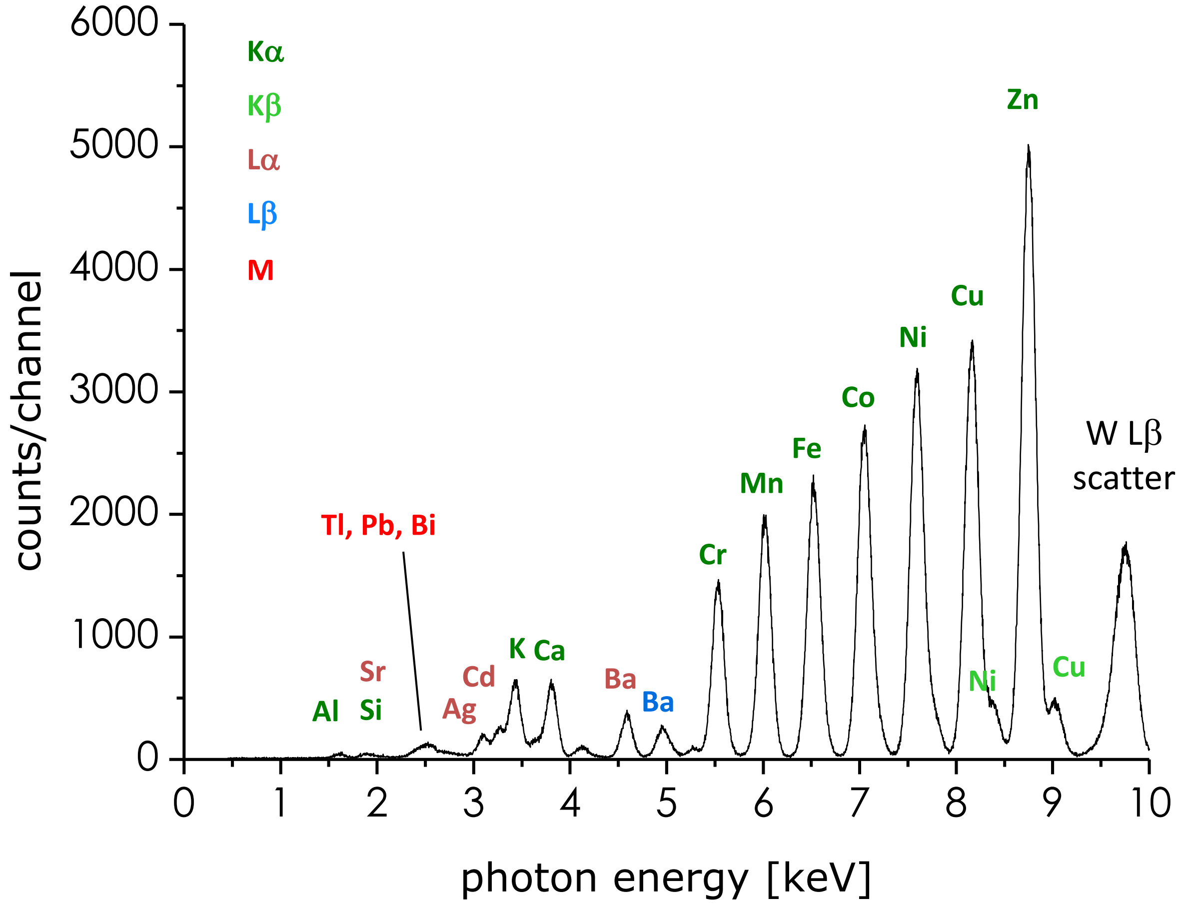
ADC

X-Ray Fluorescence analysis

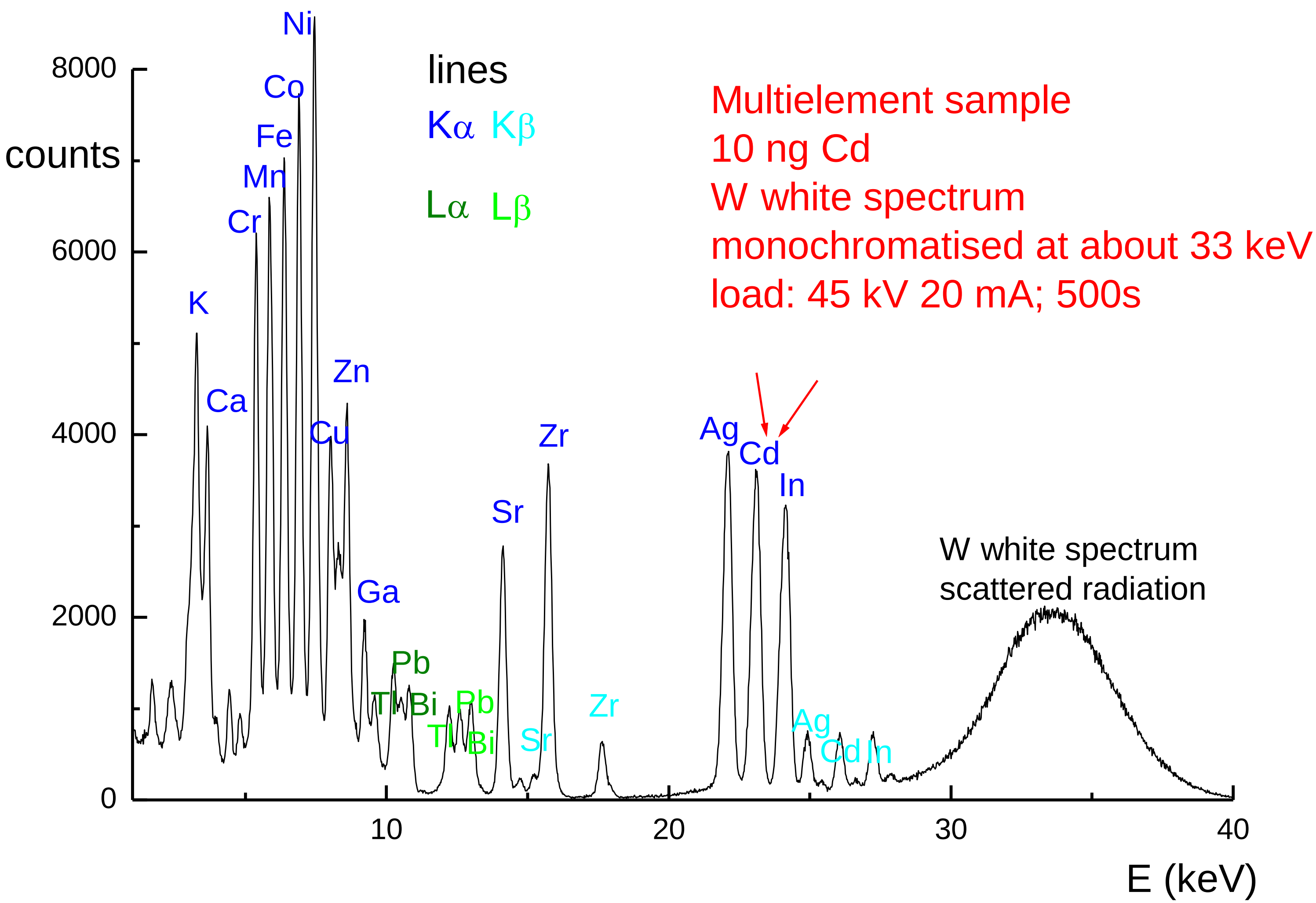


Element	Concentration	Uncertainty
Ca	51,316	0,500
Cr	46,281	0,239
Mn	48,436	0,226
Fe	48,590	0,197
Co	50,803	0,179
Ni	52,852	0,164
Cu	50,330	0,146
Zn	52,675	0,136
Ga	50,000	0
Sr	51,947	0,087
Ba	48,295	0,501
Tl	56,445	0,129
Pb	43,545	0,108
Bi	46,477	0,109
Ag	56,982	2,160
Cd	56,722	2,398

X-Ray Fluorescence analysis

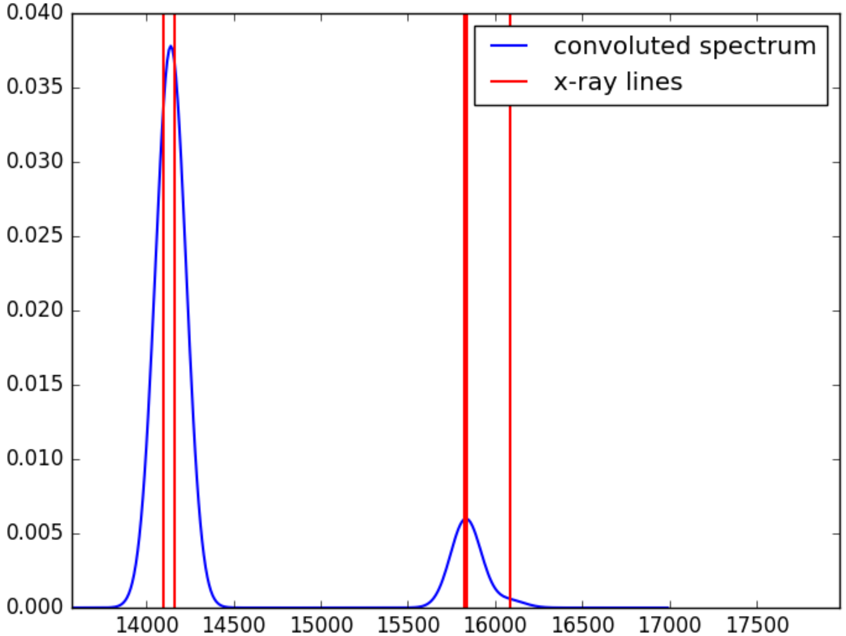


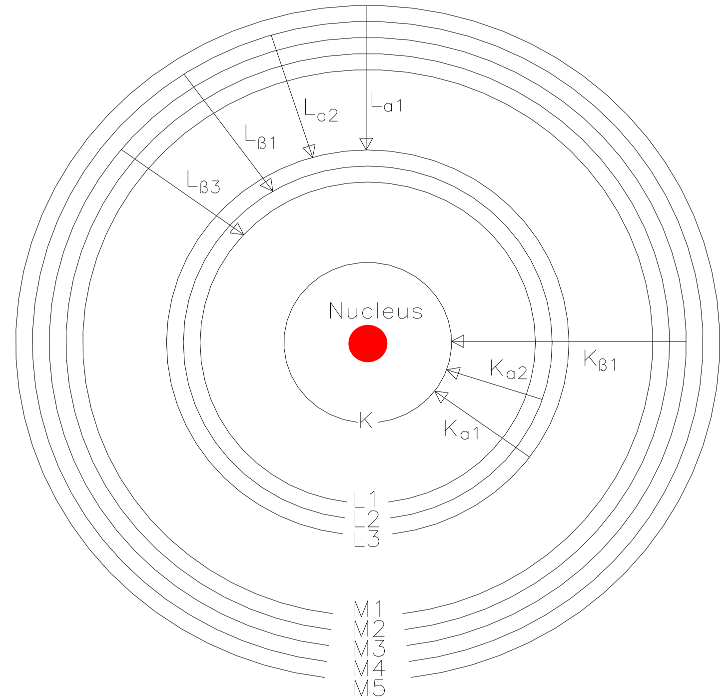
X-Ray Fluorescence analysis



X-Ray line families

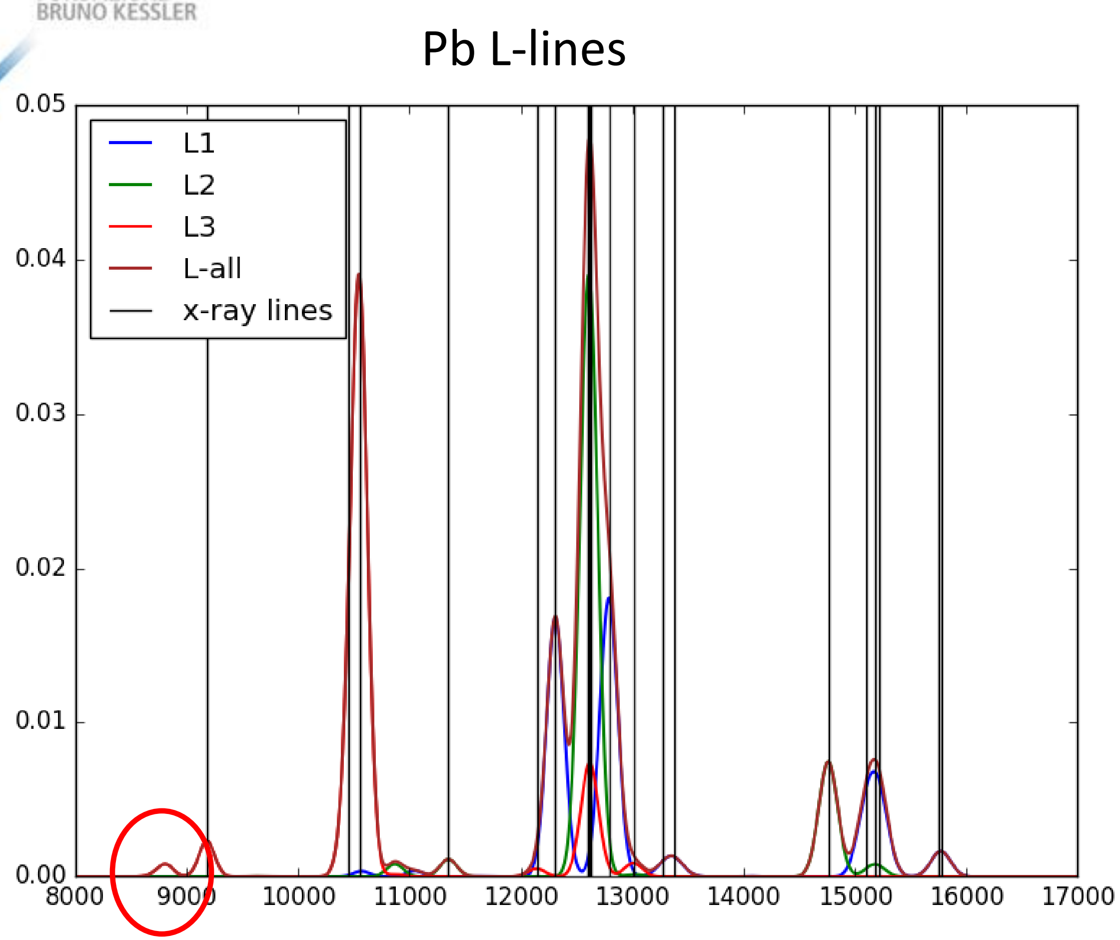
Sr-K lines

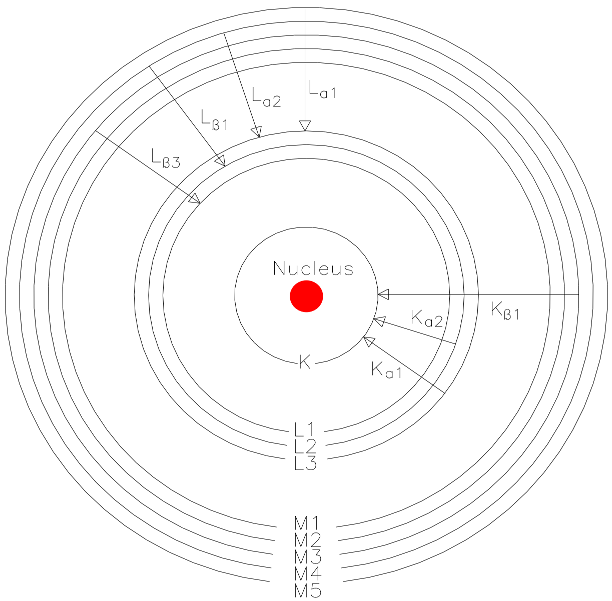




Siegbahn	IUPAC	Siegbahn	IUPAC
$K\alpha_1$	K-L3	$L\alpha_1$	L3-M5
$K\alpha_2$	K-L2	$L\alpha_2$	L3-M4
$K\beta_1$	K-M3	$L\beta_1$	L2-M4
$K\beta_2$	K-N2,N3	$L\beta_2$	L3-N5
$K\beta_3$	K-M2	$L\beta_3$	L1-M3
		$L\beta_4$	L1-M2

X-Ray line families

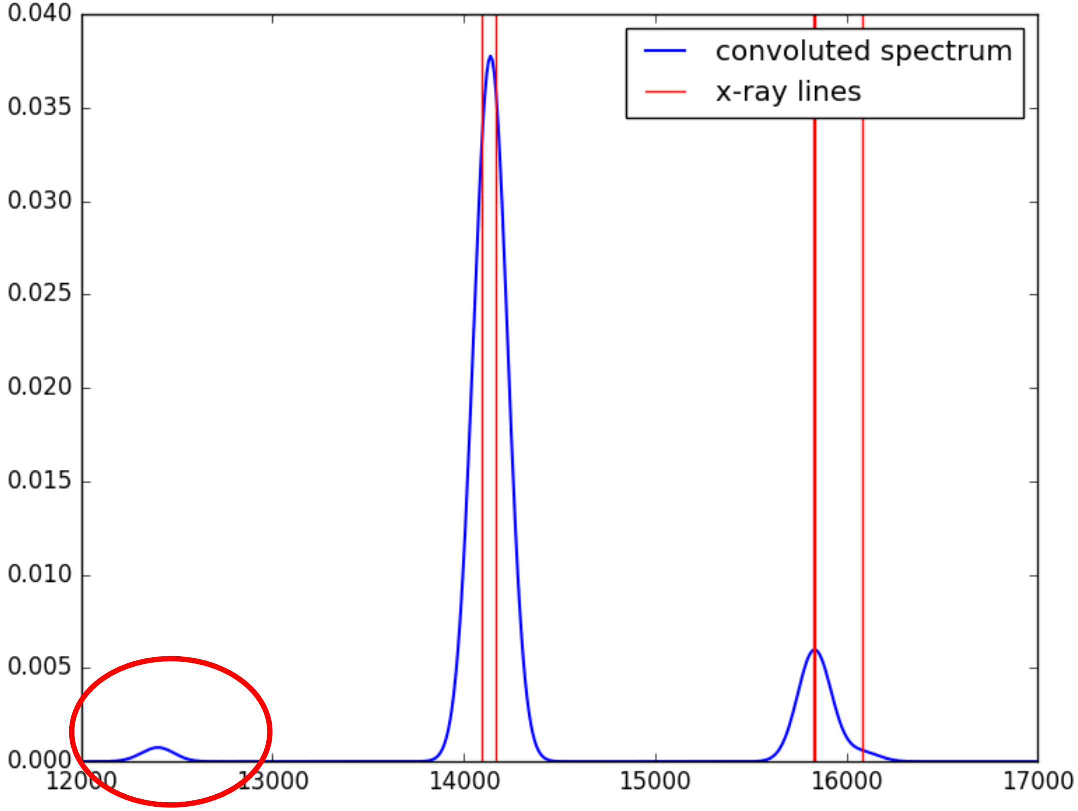




Siegbahn	IUPAC	Siegbahn	IUPAC
$K\alpha_1$	K-L3	$L\alpha_1$	L3-M5
$K\alpha_2$	K-L2	$L\alpha_2$	L3-M4
$K\beta_1$	K-M3	$L\beta_1$	L2-M4
$K\beta_2$	K-N2,N3	$L\beta_2$	L3-N5
$K\beta_3$	K-M2	$L\beta_3$	L1-M3
		$L\beta_4$	L1-M2

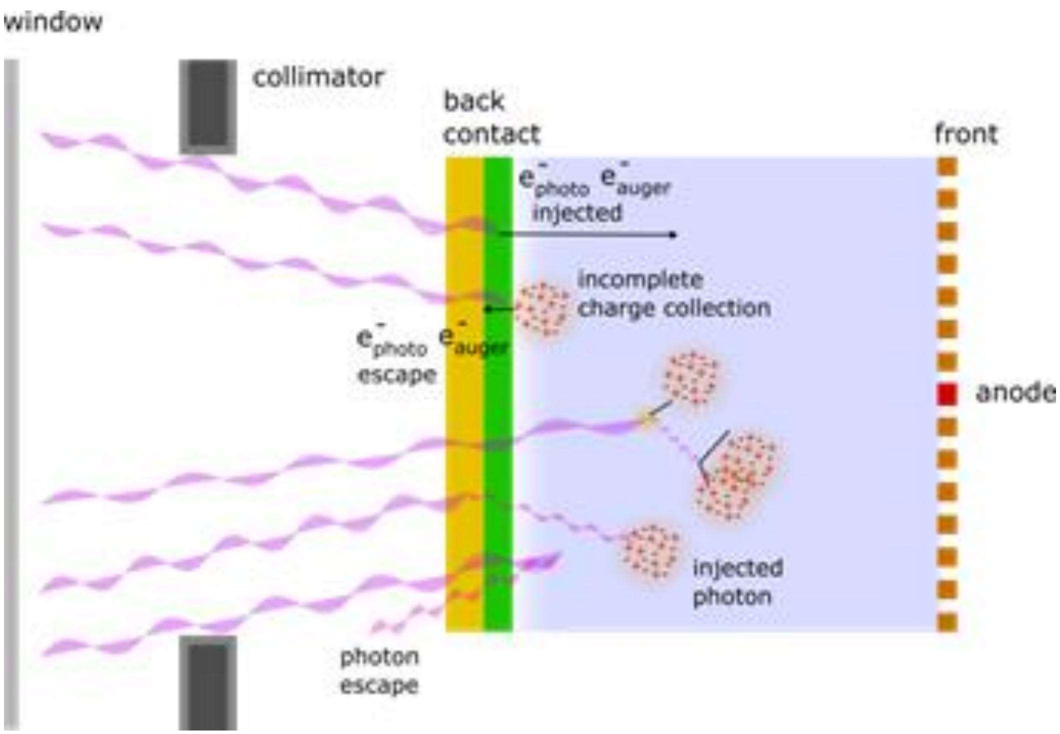
X-Ray line families

Sr-K lines



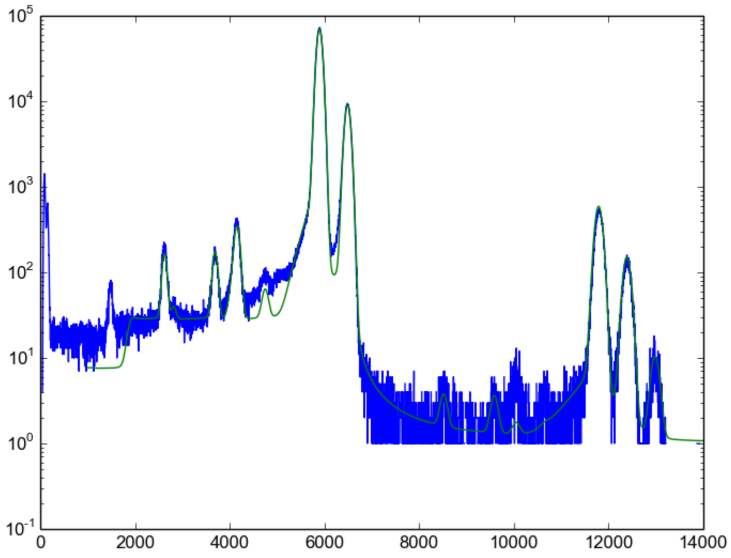
Siegbahn	IUPAC	Siegbahn	IUPAC
$K\alpha_1$	K-L3	$L\alpha_1$	L3-M5
$K\alpha_2$	K-L2	$L\alpha_2$	L3-M4
$K\beta_1$	K-M3	$L\beta_1$	L2-M4
$K\beta_2$	K-N2,N3	$L\beta_2$	L3-N5
$K\beta_3$	K-M2	$L\beta_3$	L1-M3
		$L\beta_4$	L1-M2

EDS detector



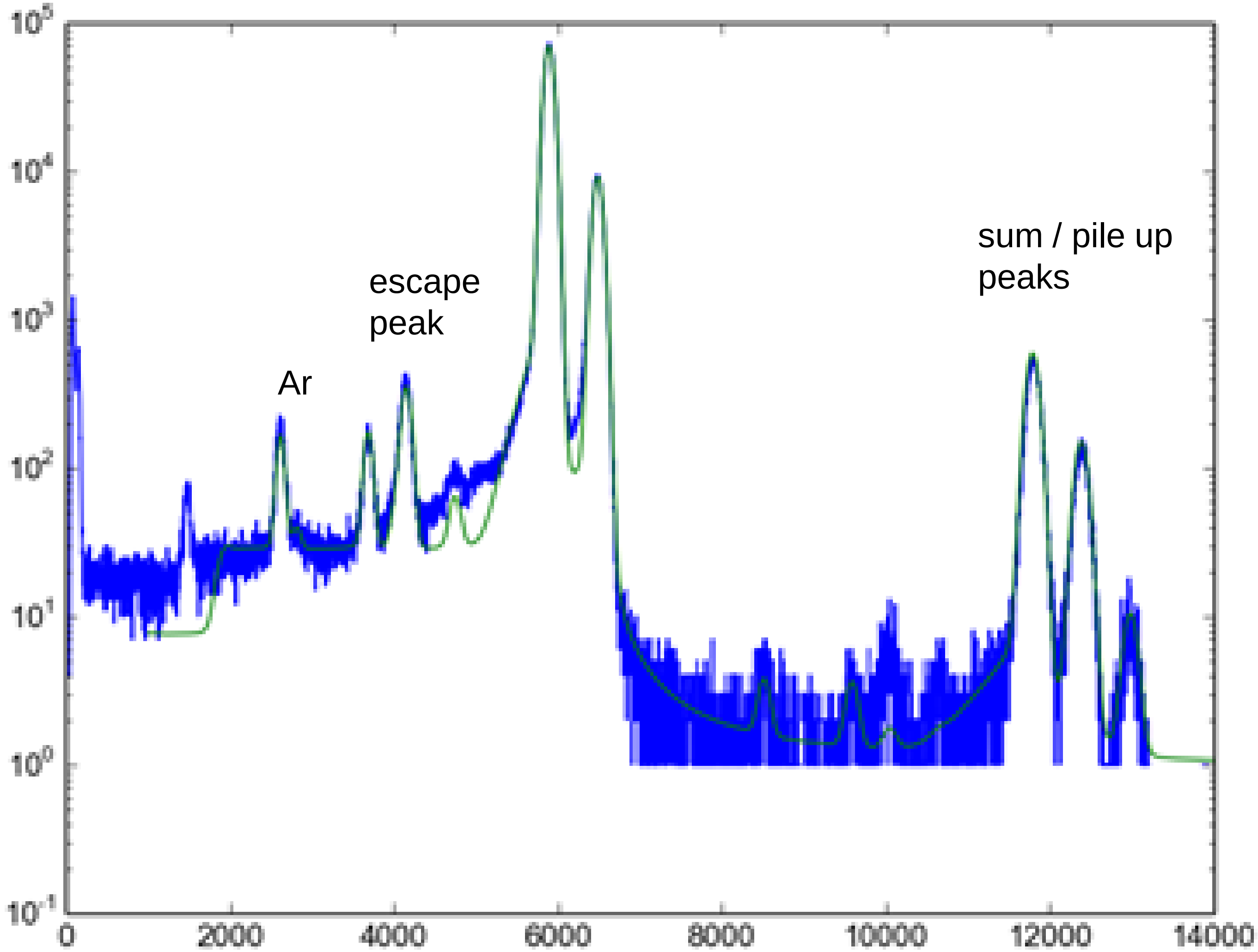
$$\epsilon_{E_{\zeta j k}}$$

detector efficiency + response

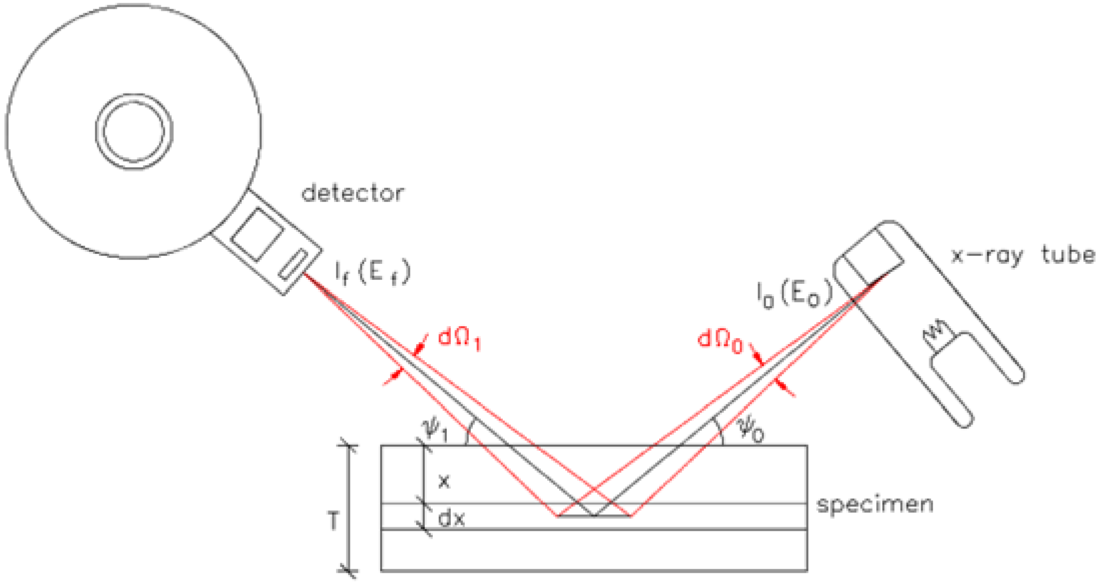


Modelling the response function of energy dispersive X-ray spectrometers with silicon detectors
F. Scholze, and M. Procop

Detector artefacts / ‘environmental’ artefacts



X-Ray Fluorescence – intensity - Sherman equation



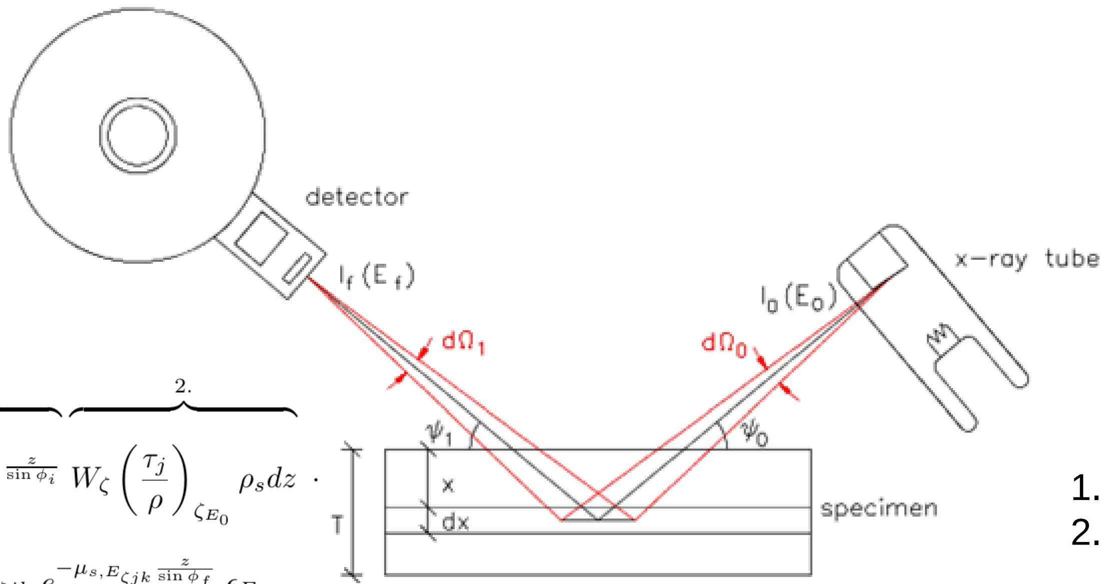
$$I_0\, G_0\, G_1$$

geometrical factors and primary flux form the element independent proportionality constant

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

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

X-Ray Fluorescence – intensity - Sherman equation



$$dI_{\zeta jk} \propto \overbrace{e^{-\mu_{s,E_0}\frac{z}{\sin\phi_i}}}^{1.}\ \overbrace{W_\zeta \left(\frac{\tau_j}{\rho}\right)_{\zeta_{E_0}} \rho_s dz}^{2.} \cdot$$

$$\cdot\ \underbrace{\omega_{\zeta j}}_{3.}\ \underbrace{p_{\zeta jk}}_{4.}\ \underbrace{e^{-\mu_{s,E_{\zeta jk}}\frac{z}{\sin\phi_f}}}_{5.}\ \underbrace{\epsilon_{E_{\zeta jk}}}_{6.}$$

$$I_0\, G_0\, G_1$$

geometrical factors and primary flux form the element independent proportionality constant

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

$$I_{\zeta jk\, layer} \propto W_\zeta \left(\frac{\tau_j}{\rho}\right)_{\zeta_E} \rho_s\, \omega_{\zeta j} p_{\zeta jk} \cdot$$

$$\cdot\ \frac{1 - e^{-\left(\frac{\mu_{s,E_{\zeta jk}}}{\sin\phi_f} + \frac{\mu_{s,E}}{\sin\phi_i}\right)T}}{\frac{\mu_{s,E_{\zeta jk}}}{\sin\phi_f} + \frac{\mu_{s,E}}{\sin\phi_i}}$$

Integration over thickness

X-Ray Fluorescence – intensity - Sherman equation

$$I_{\zeta jk} = I_0 \, G \, S_{\zeta jk} \, \rho_s \, W_\zeta \int_{\mathrm{E}_{edge}}^{\mathrm{E}_{max}} \int_0^{\mathrm{t}} \exp\left[-\left(\frac{\mu_{s,E_0}}{\sin\phi_i} + \frac{\mu_{s,E_{\zeta jk}}}{\sin\phi_f}\right) z\right] dz \, dE$$

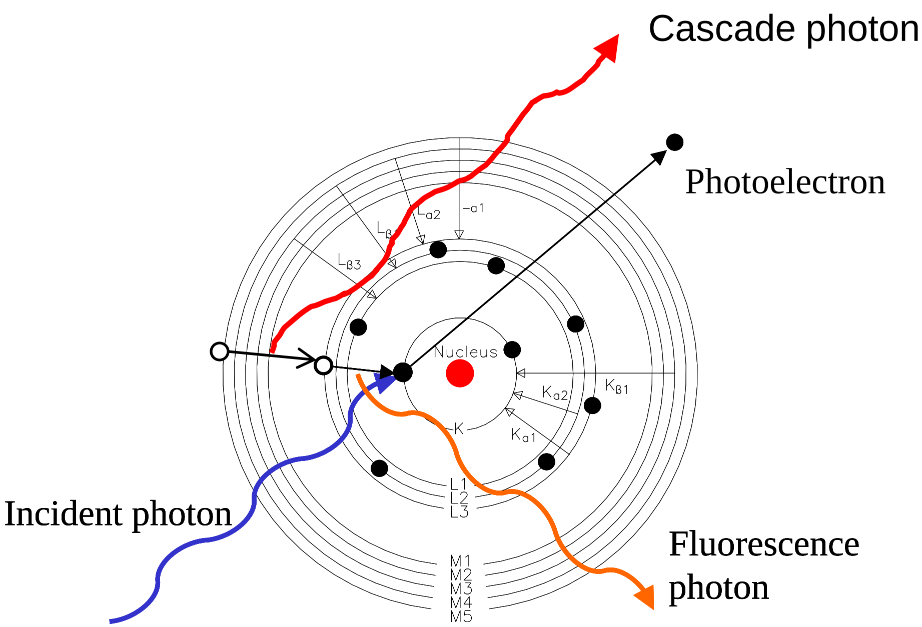
Monochromatic

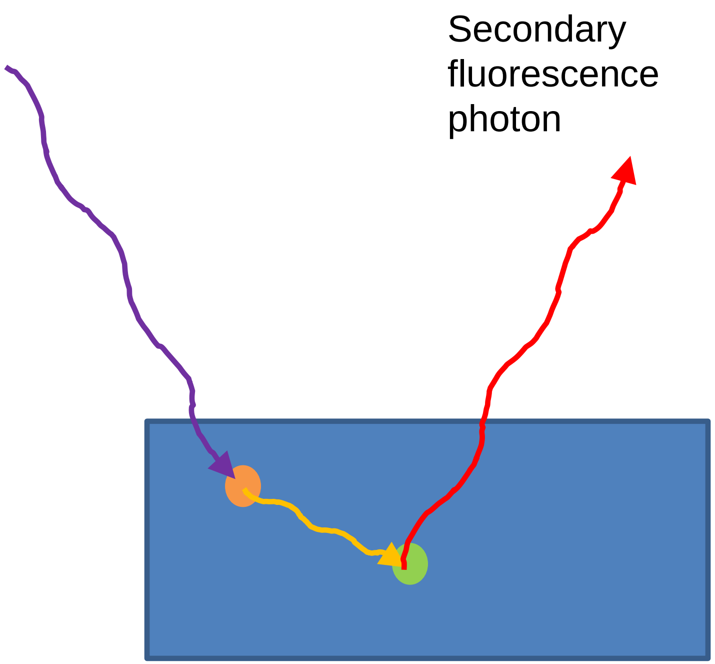
$$I_{\zeta jk} = I_0 \, G \, S_{\zeta jk} \, \rho_s \, W_\zeta \int_0^{\mathrm{t}} \exp\left[-\left(\frac{\mu_{s,E_0}}{\sin\phi_i} + \frac{\mu_{s,E_{\zeta jk}}}{\sin\phi_f}\right) z\right] dz$$

$$= I_0 \, G \, S_{\zeta jk} \, \rho_s \, W_\zeta \frac{1 - \exp\left[-\left(\frac{\mu_{s,E_0}}{\sin\phi_i} + \frac{\mu_{s,E_{\zeta jk}}}{\sin\phi_f}\right) t\right]}{\left(\frac{\mu_{s,E_0}}{\sin\phi_i} + \frac{\mu_{s,E_{\zeta jk}}}{\sin\phi_f}\right)}$$

$$\left(\frac{\mu}{\rho}\right)_{sample} = \sum_\zeta W_\zeta \left(\frac{\mu}{\rho}\right)_\zeta$$

Fluorescence enhancement, secondary fluorescence



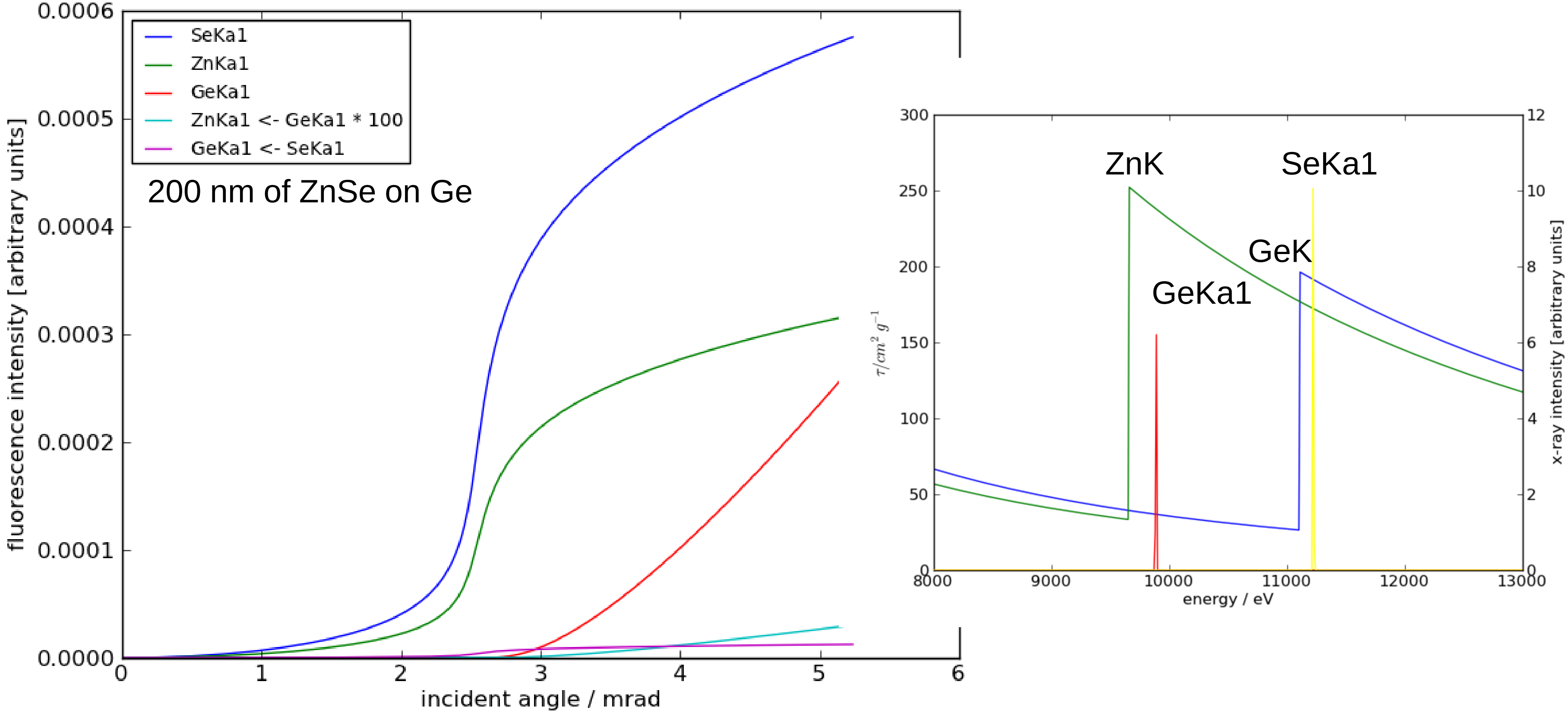


Fluorescence enhancement, secondary fluorescence

J. Appl. Phys. **75**, 2026 (1994); http://dx.doi.org/10.1063/1.356303 (*3 pages*)

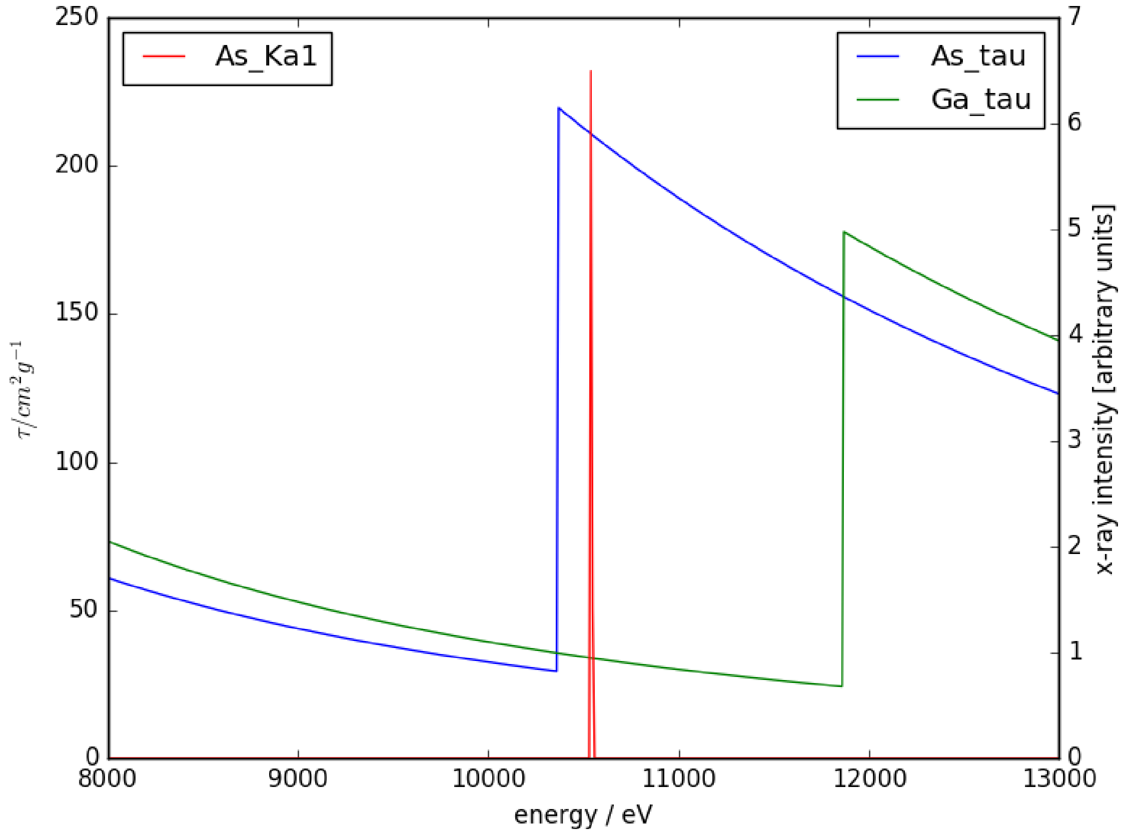
Molecular beam epitaxial growth of single domain ZnSe on Ge

L. K. Li, Y. Wang, M. Jurkovic, and W. I. Wang



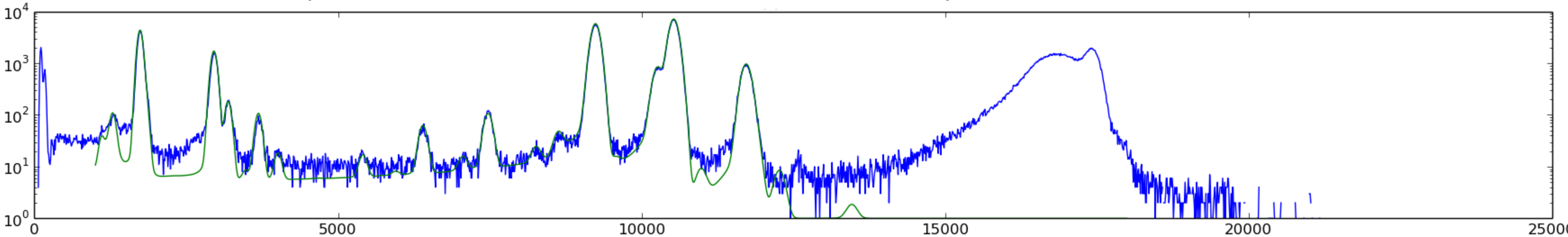
Fluorescence enhancement, secondary fluorescence

GaAs

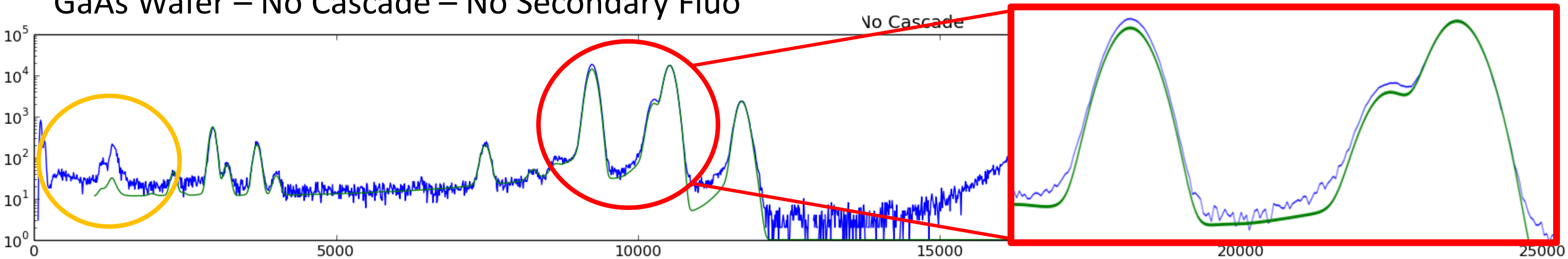


Fluorescence enhancement, secondary fluorescence

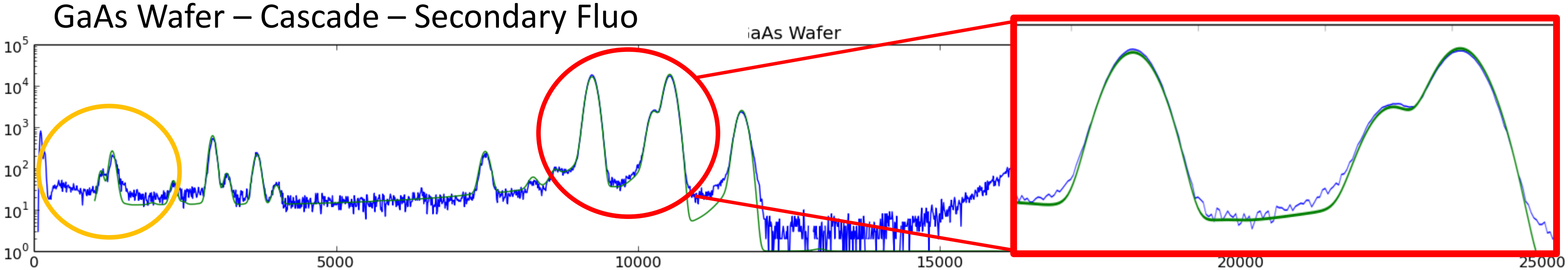
GaAs solution deposited on silicon – Cascade – No Secondary Fluo



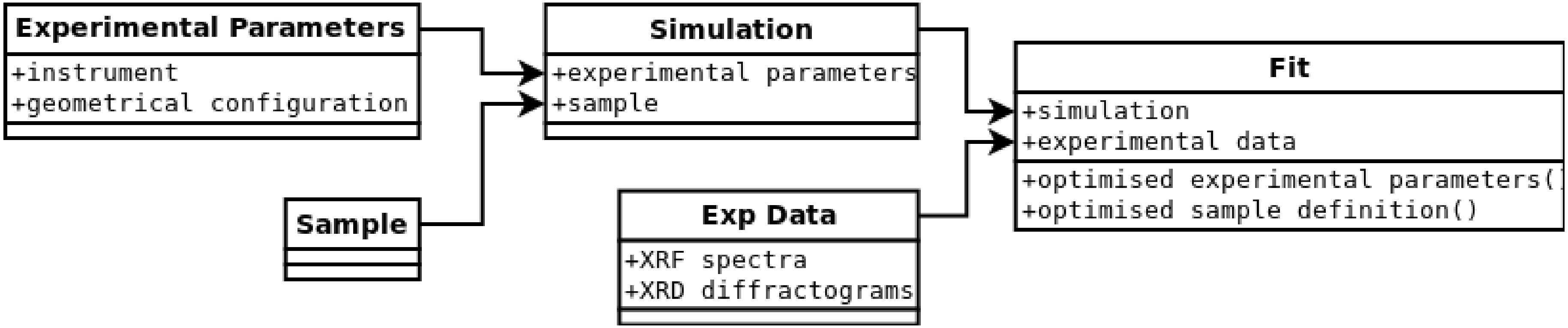
GaAs Wafer – No Cascade – No Secondary Fluo



GaAs Wafer – Cascade – Secondary Fluo



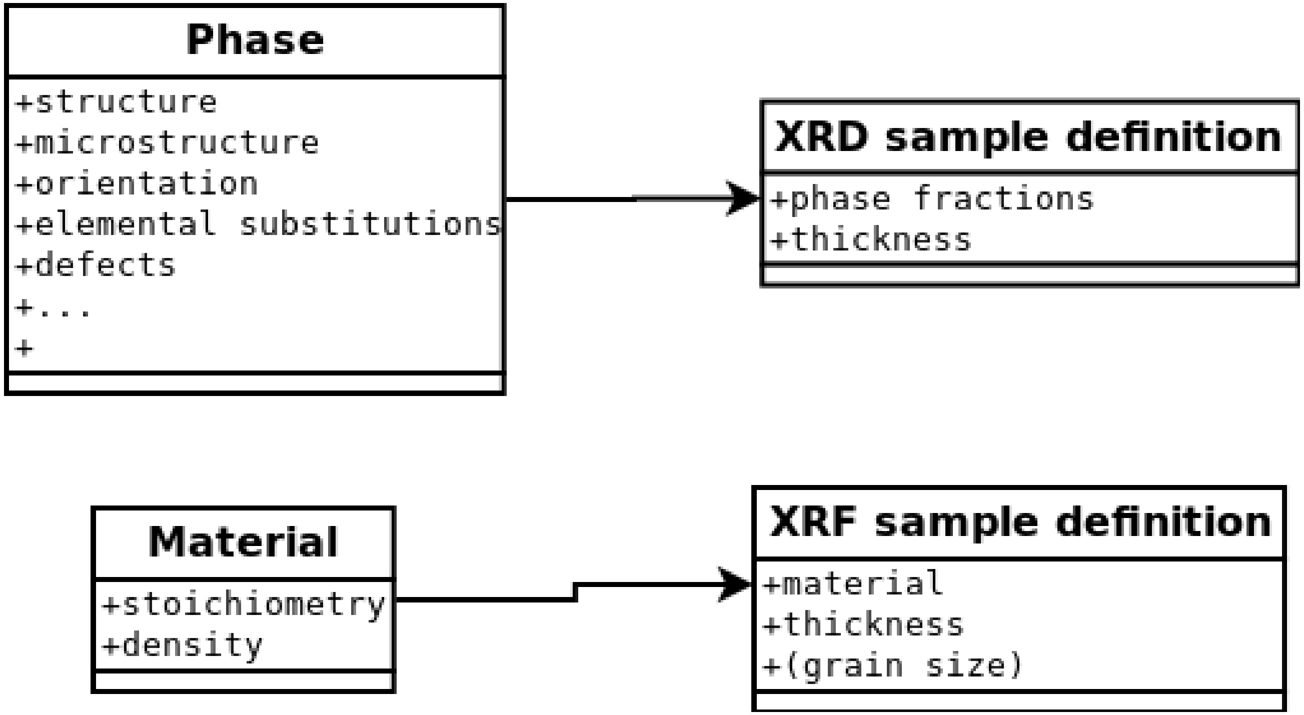
Data analysis XRD vs XRF



XRD : Rietveld

XRF : Fundamental parameters method

Data analysis XRD vs XRF



In MAUD:
the XRD definitions are obviously followed, since they are contain more information:

from the XRD definition you can derive the XRF one, not the other way around

Instrumental parameters

XRF: energy, intensity fraction

XRD: wavelength, intensity fraction

$$\lambda = \frac{hc}{E}$$

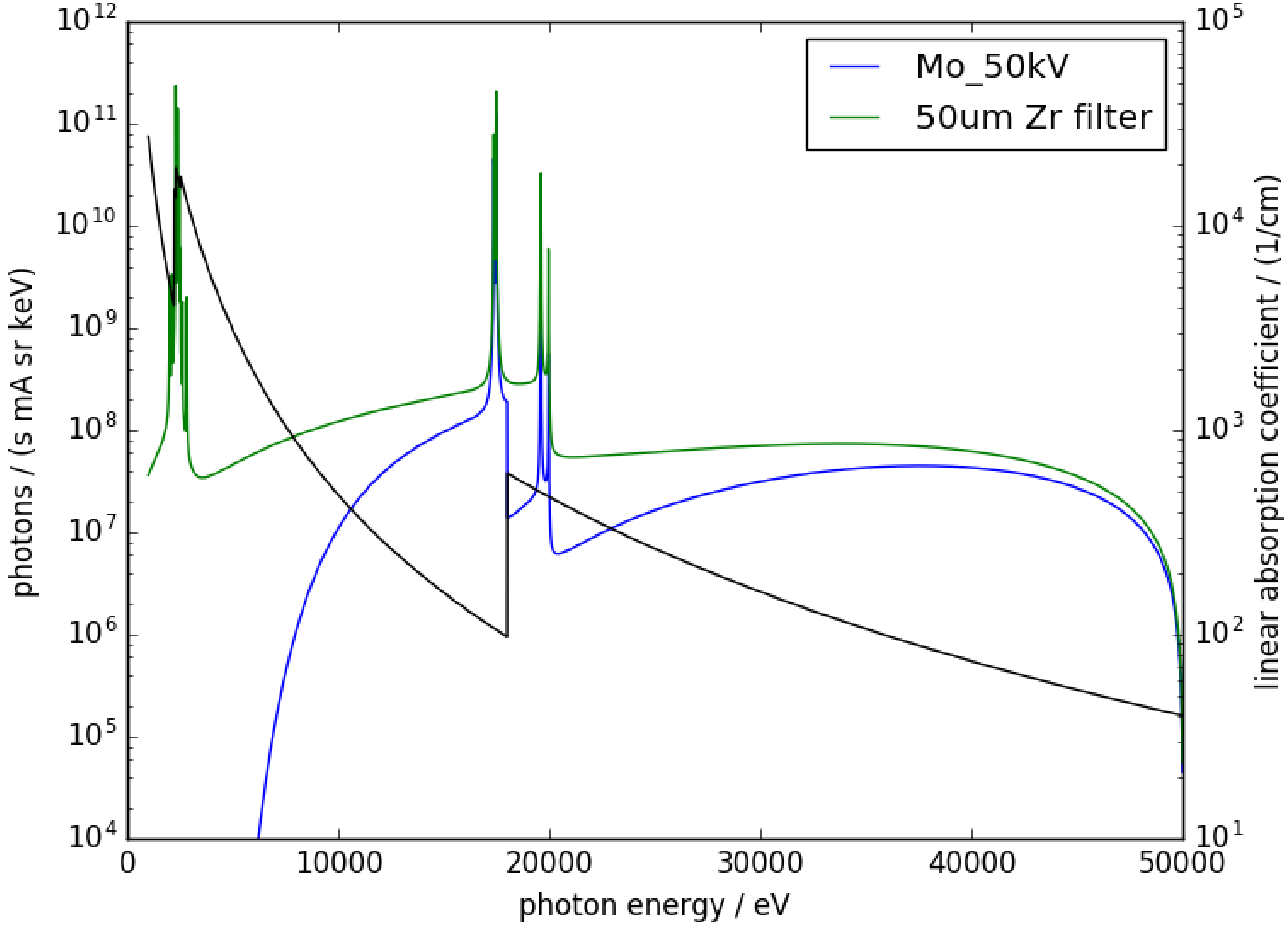
$$\lambda(\text{Å}) = \frac{12.3984}{\text{E(eV)}}$$

In MAUD:

One or multiple wavelengths can be indicated with intensity fraction

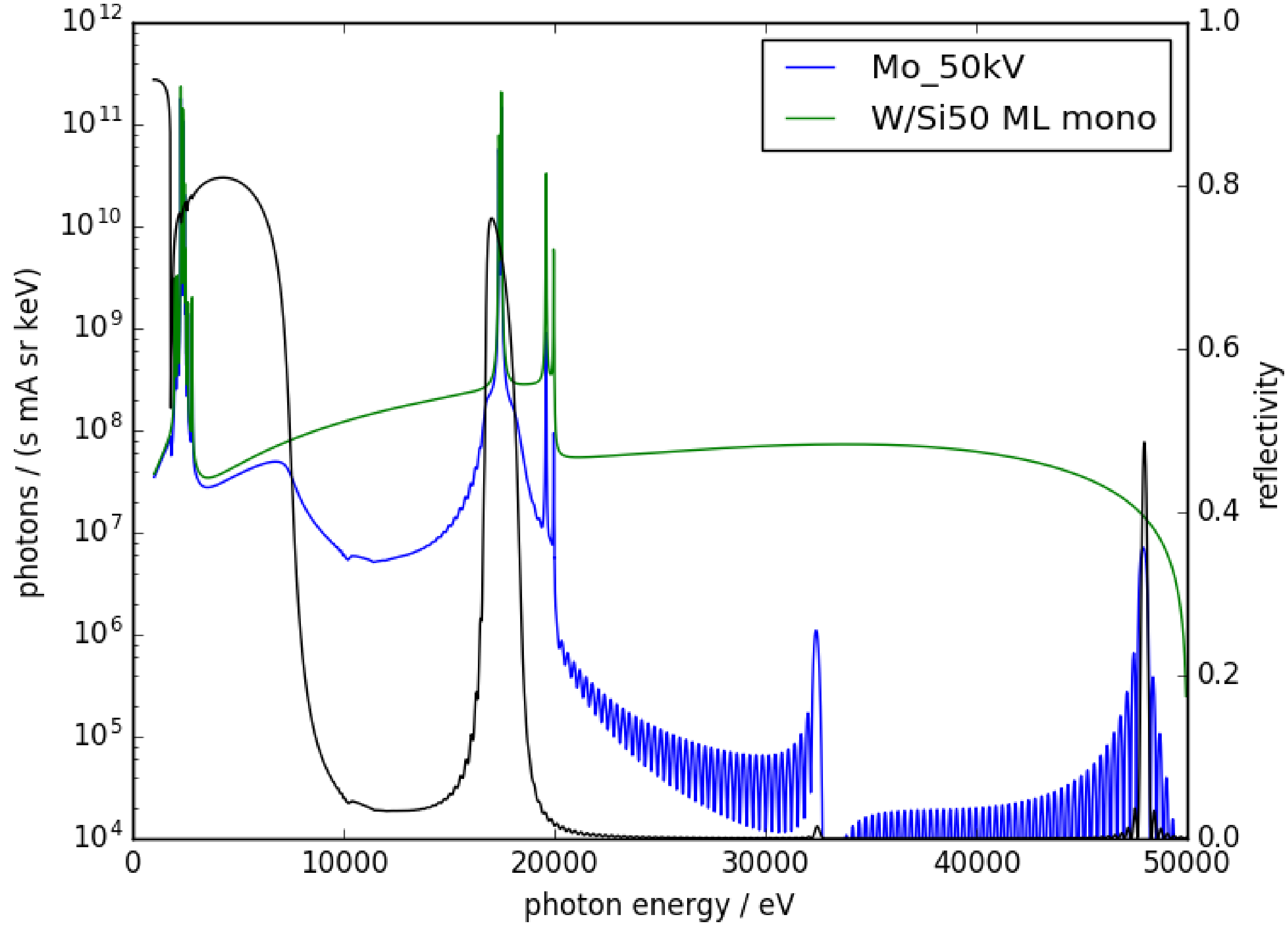
Integration over different energies/wavelengths done numerically

Primary radiation – x-ray tube



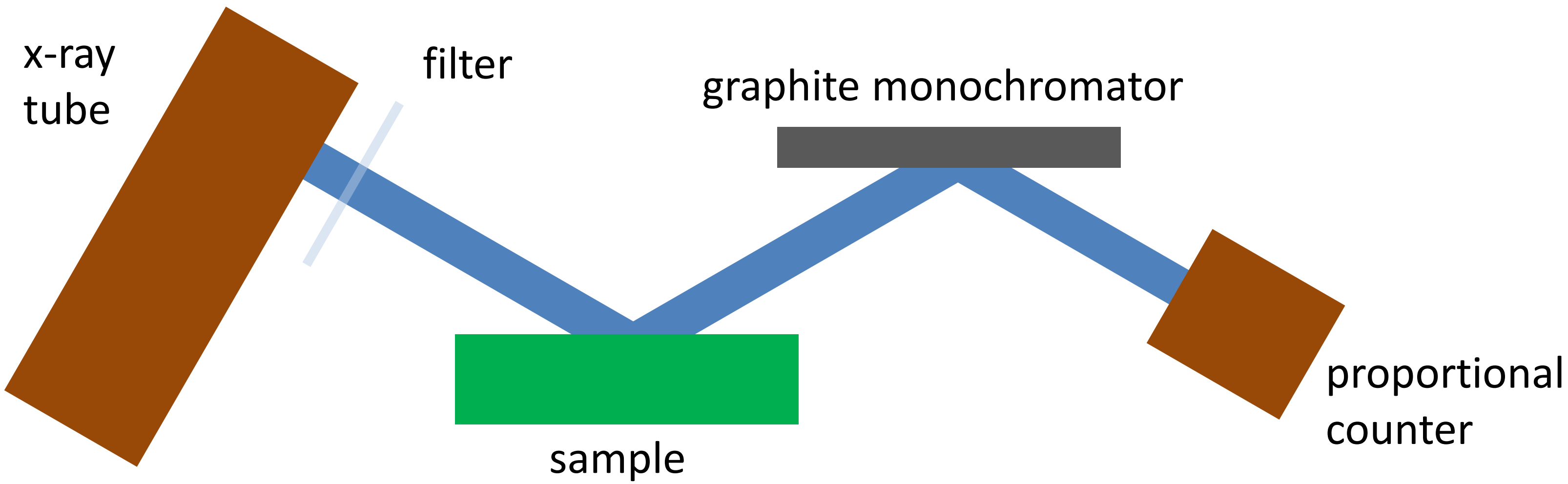
Tube spectrum and filtered spectrum automatically calculated in MAUD

Primary radiation – x-ray tube



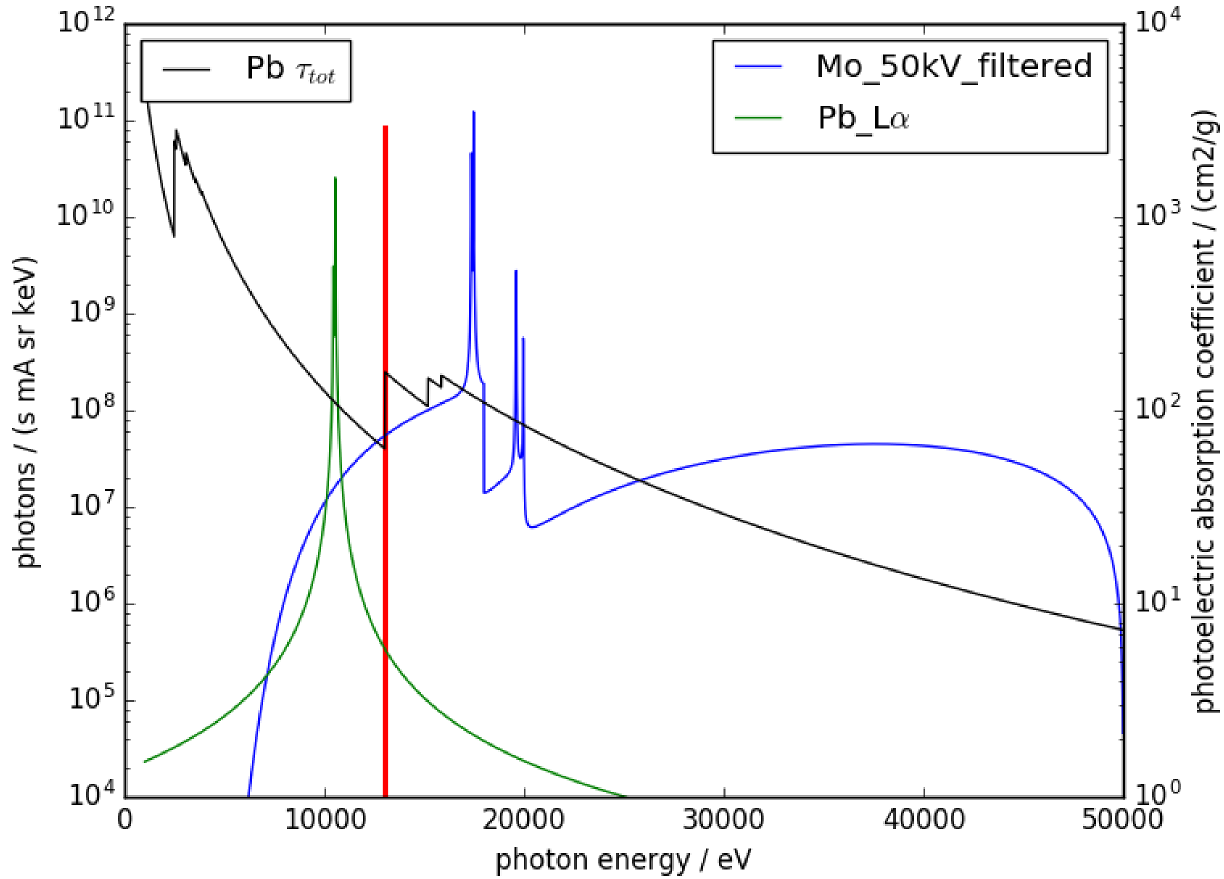
Tube spectrum and filtered spectrum automatically calculated in MAUD

Primary radiation – x-ray tube



XRF and XRD signals related to different part of the X-ray primary beam
In MAUD: defined separately, hence taken into account

X-Ray Fluorescence – intensity - Sherman equation

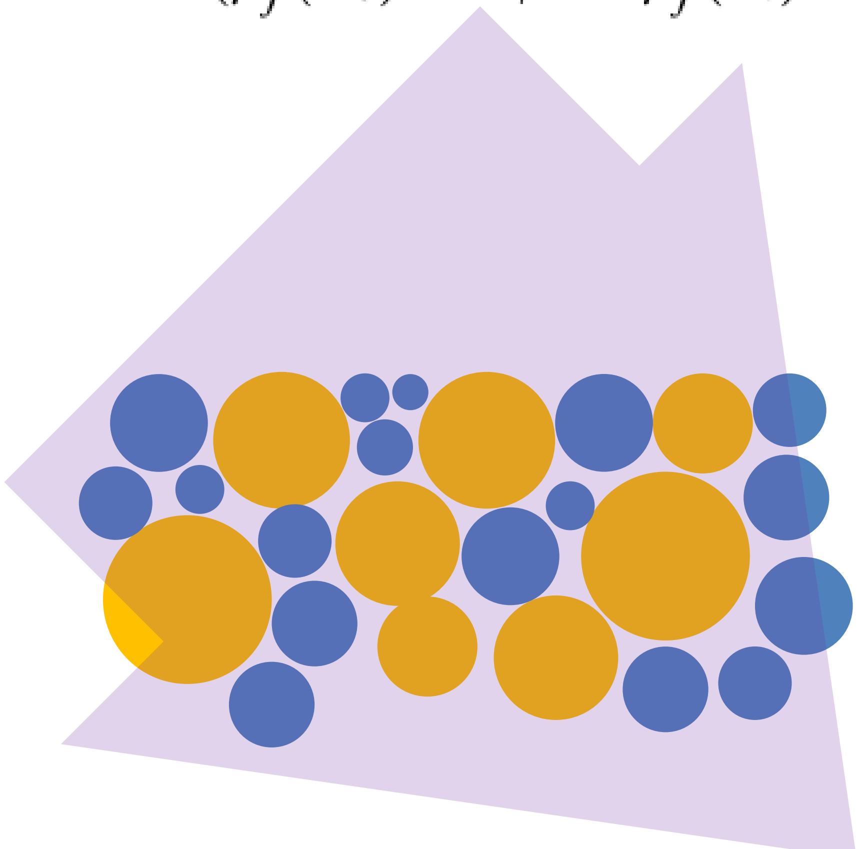


$$I_{\zeta jk\,layer} \propto \int_{E_{edge}}^{E_{max}} W_\zeta \left(\frac{\tau_j}{\rho}\right)_{\zeta_E} \rho_s\, \omega_{\zeta j} p_{\zeta jk} \cdot$$

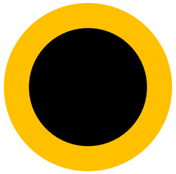
$$\cdot \frac{1 - e^{-\left(\frac{\mu_{s,E_{\zeta jk}}}{\sin\phi_f} + \frac{\mu_{s,E}}{\sin\phi_i}\right)T}}{\frac{\mu_{s,E_{\zeta jk}}}{\sin\phi_f} + \frac{\mu_{s,E}}{\sin\phi_i}} \mathrm{dE}$$

Grain size effect in XRF

$$F_i = \frac{1 - \exp[-(\mu_f^*(E_0)\csc\psi_1 + \mu_f^*(E_i)\csc\psi_2)a_r]}{(\mu_f^*(E_0)\csc\psi_1 + \mu_f^*(E_i)\csc\psi_2)a_r}$$



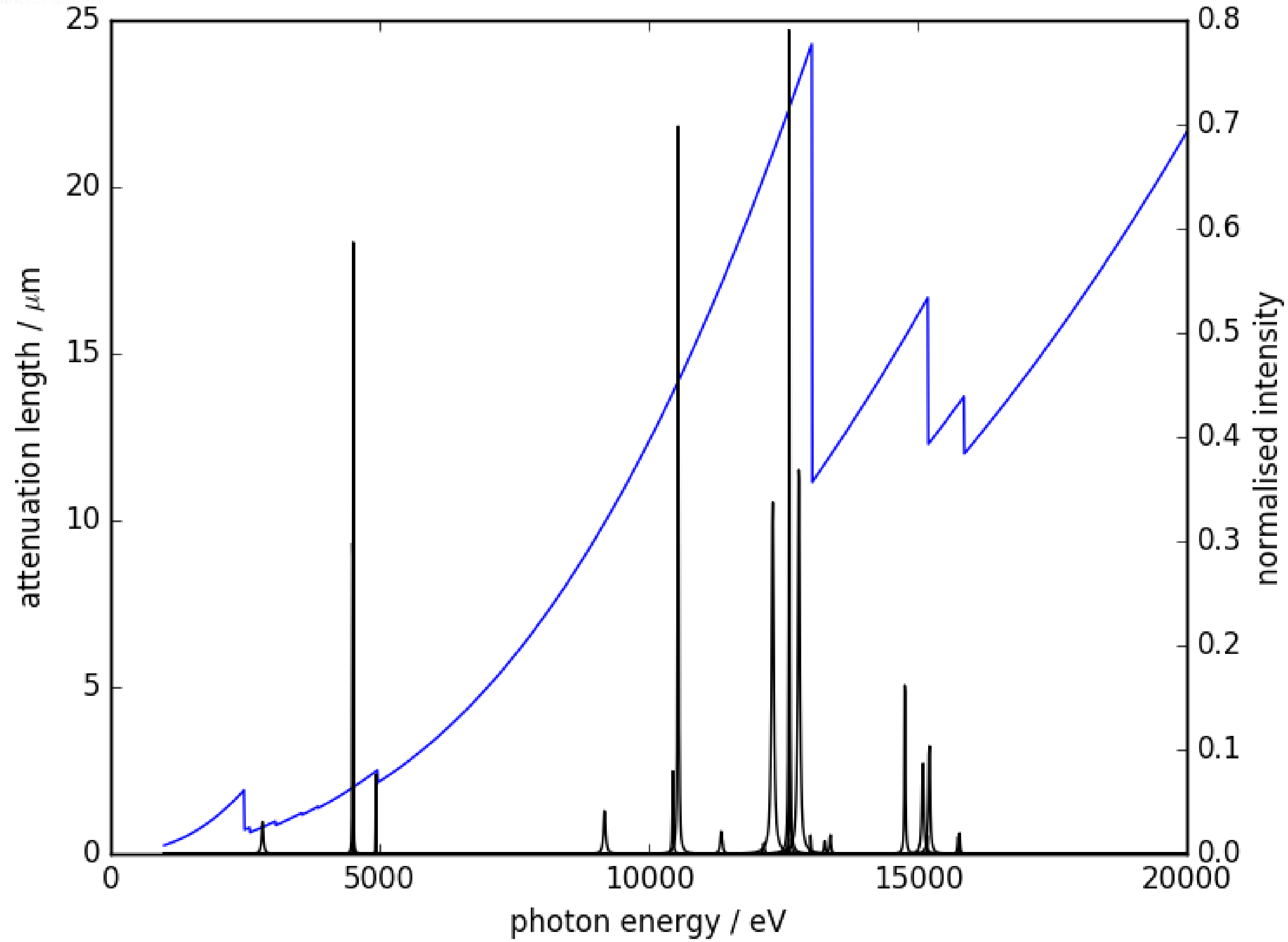
μ* = linear absorption coeficient

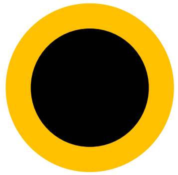


a_r = radiometric particle diameter
a = geometric particle diameter

Similar to Brindley correction, but not quite the same:
In Maud? Work in progress

Grain size effect in XRF





PbTiO3

overcome by sample preparation : fused beads
1050 deg C + lithium tetraborate (LiT or $Li_2B_4O_7$) and lithium metaborate (LiM or $LiBO_2$)
(commonly used in various proportions)

Thank you for your attention!