Interaction X-rays - Matter

Pair production
$h\nu > 1M\,eV$

Photoelectric absorption

$h\nu$ — X-rays

MATTER

$h\nu$ — Transmission

Scattering
$h\nu' < h\nu$ Compton
$h\nu$ Thomson

Decay processes
$h\nu_f$
Fluorescence   Auger electrons
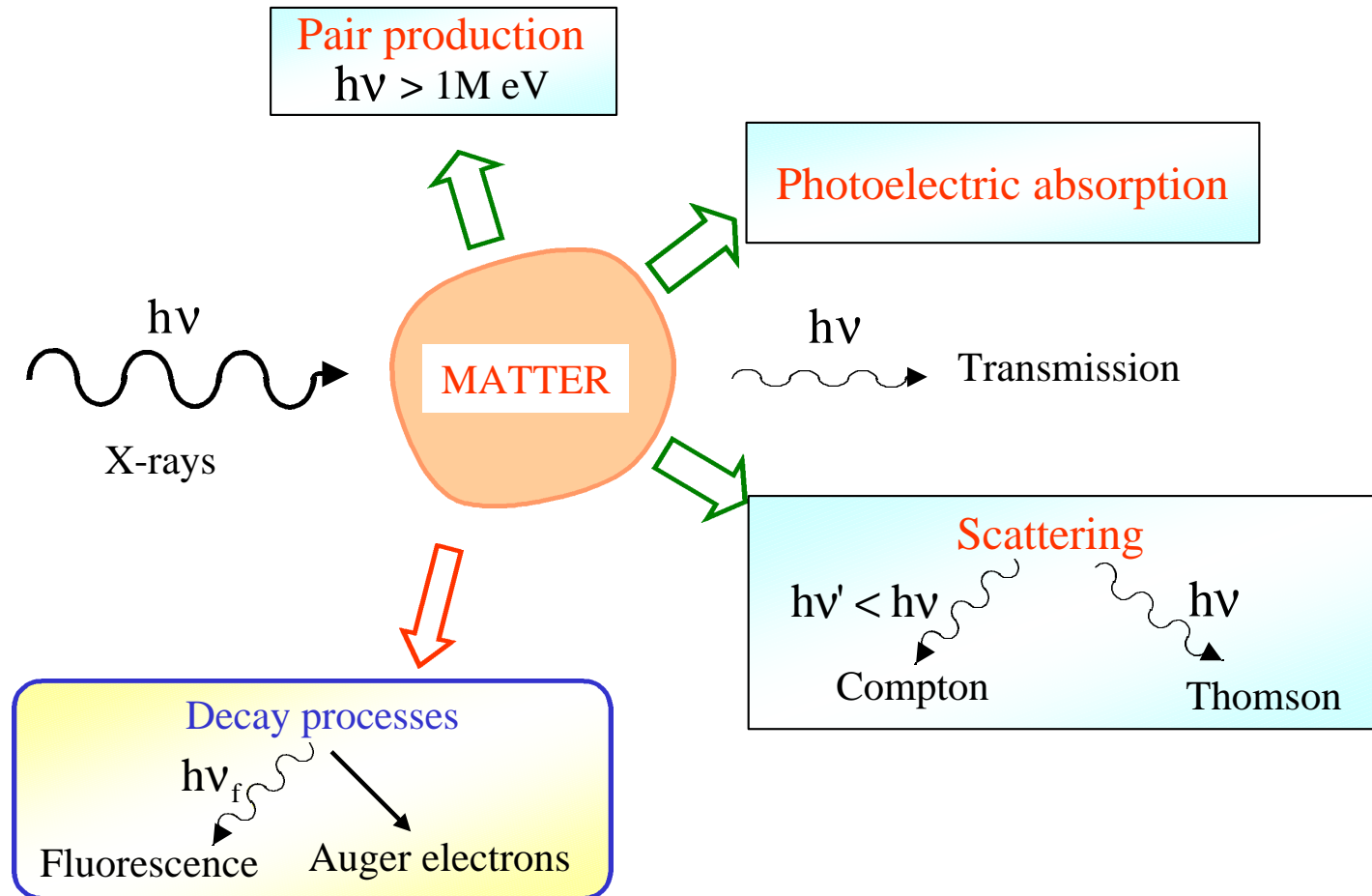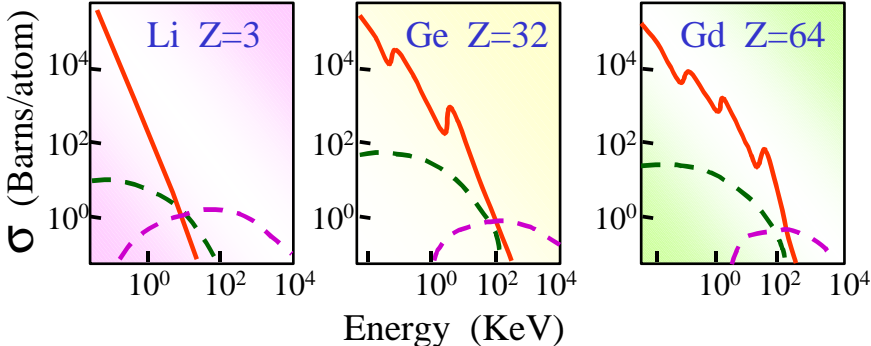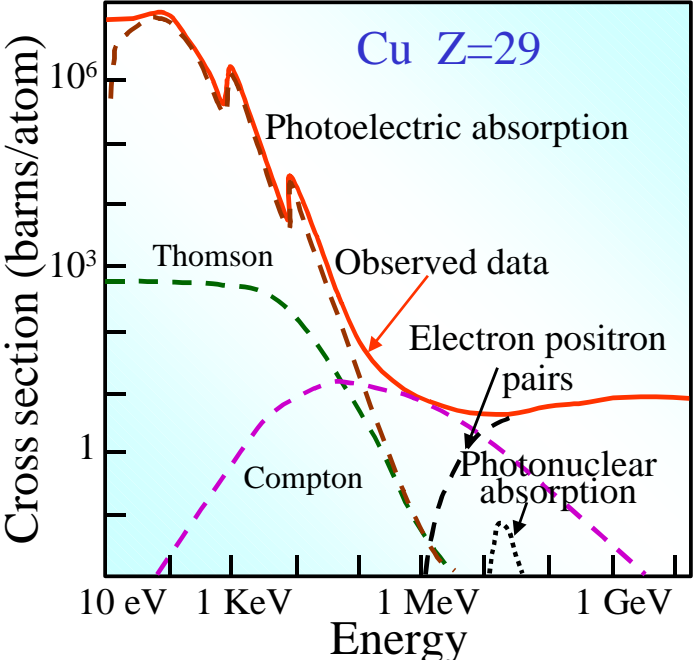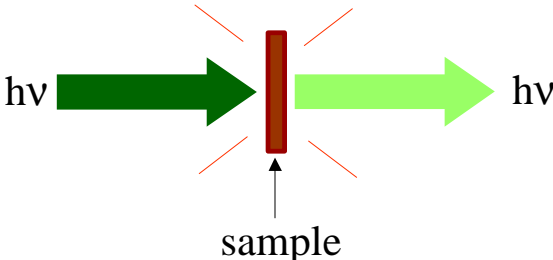
Primary competing processes and some radiative and non-radiative decay processes

X-ray attenuation: atomic cross section

hν → sample → hν

Cu Z=29

Photoelectric absorption

Thomson

Observed data

Electron positron pairs

Compton

Photonuclear absorption

Cross section (barns/atom)

10^6

10^3

1

10 eV   1 KeV   1 MeV   1 GeV

Energy

Li Z=3

Ge Z=32

Gd Z=64

σ (Barns/atom)

10^4

10^2

10^0

10^0 10^2 10^4

Energy (KeV)

Interactions between x-rays and matter

The fundamental interactions between matter and x-rays having energy less than 1 MeV are:
- elastic, coherent or Rayleigh scattering
- inelastic, incoherent or Compton scattering
- photoelectric absorption

They all contribute to the attenuation of intensity when an x-ray beam crosses matter. The phenomenon is described by the Beer-Lambert law
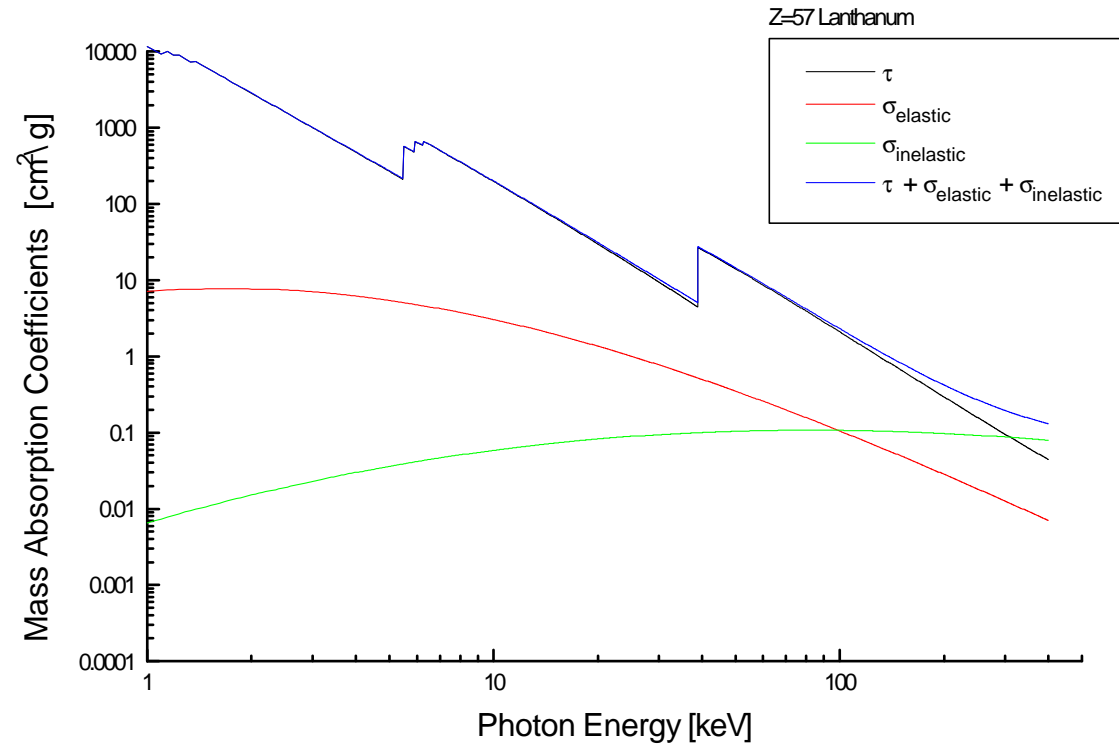
$$I(t) = I_0 \, exp \, (-\boldsymbol{m}t)$$

μ is the linear absorption coefficient. It is dependent on the energy of the radiation and specific for a certain element and it is the sum of the coefficients representing the phenomena mentioned above

$$\boldsymbol{m} = \boldsymbol{t} + \boldsymbol{s}_{elastic} + \boldsymbol{s}_{inelastic}$$

$\boldsymbol{t}$ the photoelectric linear absorption coefficient, is by far the most important at low energies

Absorption coefficient

Photoelectric mass absorption, coherent scattering, incoherent scattering coefficients of Lanthanum (Z=57) versus energy of the incident photon.

In literature the mass absorption coefficient $\mu_m = \mu/\rho$ is more likely to be found.

The coefficient for a compound C is calculated taking into account the weight fractions W_i of the elements in the sample considered

$$\left(\frac{m}{r}\right)_C = \sum_i W_i \left(\frac{m}{r}\right)_i = \sum_i W_i \left(\left(\frac{t}{r}\right)_i + \left(\frac{s_{el}}{r}\right)_i + \left(\frac{s_{in}}{r}\right)_i \right)$$

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Elastic scattering

It represents the collision of a photon with a tightly bound electron leading to an outgoing photon with a different direction but the same energy.
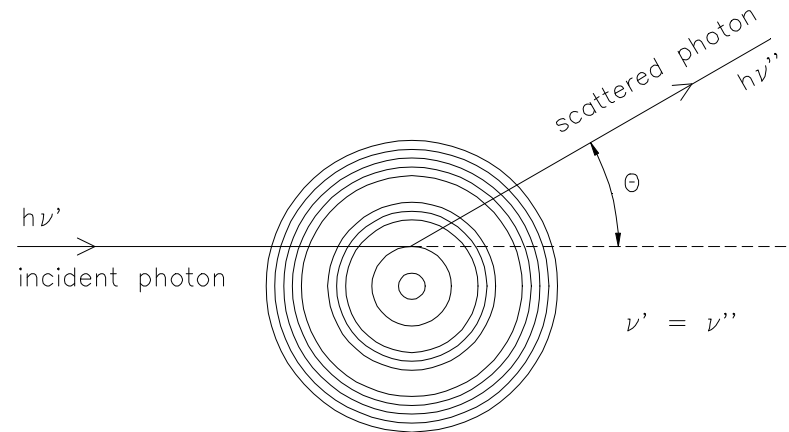
Rayleigh scattering

Rayleigh scattering occurs mostly at the low energies and for high Z materials.
The elastic scattering cross section is given by:

$$\frac{d\boldsymbol{s}_{el}}{d\Omega} = \frac{d\boldsymbol{s}_T}{d\Omega}\left|F(x,Z)\right|^2$$

where $\dfrac{d\boldsymbol{s}_T}{d\Omega}$ is the Thomson scattering cross section for one electron $\qquad \dfrac{d\boldsymbol{s}_T}{d\Omega} = \dfrac{r_0^2}{2}(1+\cos^2\boldsymbol{q})$

$F(x,Z)$ is the atomic form factor and $x = \dfrac{sin \dfrac{q}{2}}{l}$.

If $\vec{q} = \dfrac{2k}{\mathbf{h}} \sin \dfrac{q}{2}$ is the momentum transfer and $\vec{r}_n$ the vector from the nucleus of the atom to the nth electron we have

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

ψ_0 is the ground-state wave function of the atom

Hence with our former notation

$$F(x,Z) = 4\mathbf{p} \int_0^{\infty} r\mathbf{r}(r) \dfrac{\sin\!\left(4\mathbf{p}\ rx \right)}{4\mathbf{p}\ rx} dr$$

in which $\rho(r)$ is the total electron density.

Incident Photon Energy = 30 keV

Z=14 Si
Z=28 Ni
Z=42 Mo
Z=56 Ba
Z=70 Yb

Elastic scattering differential cross section for different elements as a function of the scattering angle and for a fixed incident photon energy equal to 30 keV.
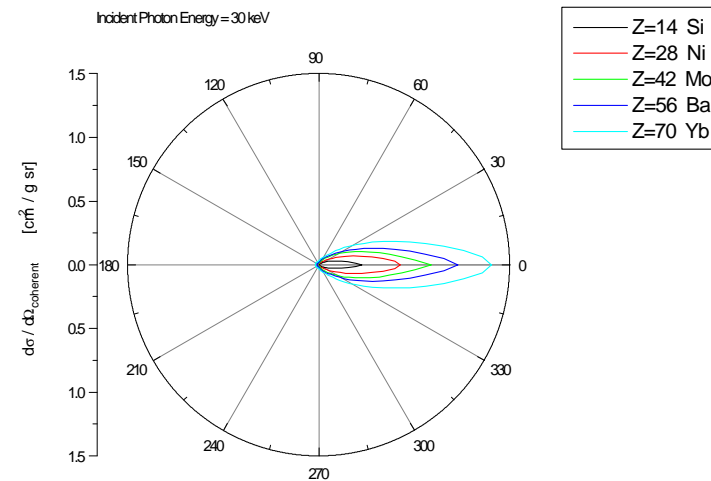
Inelastic scattering

A loosely bound or free electron hit by a photon undergoes Compton effect and the scattered photon has different direction and lower energy
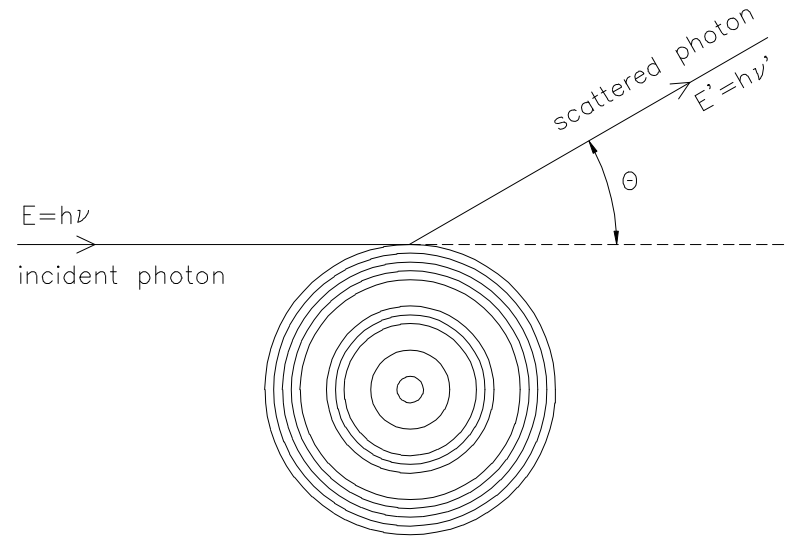
Compton scattering

The energy of the outgoing photon is

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

The differential inelastic cross section for a single free electron is given by Klein-Nishina formula

$$\frac{d\mathbf{s}_{KN}}{d\Omega} = \frac{r_0^2}{2} P(\mathbf{q}, E)$$

where $P(\mathbf{q}, E)$ is called the polarisation factor;

$$P(\mathbf{q}, E) = \frac{1}{\left(1 + \mathbf{a}(1 - \cos\mathbf{q})\right)^2}\left[1 + \cos^2\mathbf{q} + \frac{\mathbf{a}^2(1 - \cos\mathbf{q})^2}{1 + \mathbf{a}(1 - \cos\mathbf{q})}\right]$$

and $\mathbf{a} = \dfrac{E}{m_0 c^2}$. If α is very small, that is if the photon energy is much smaller than the electron rest mass, then the polarisation factor reduces to $1 + \cos^2\mathbf{q}$ and the Klein-Nishina differential cross section to the Thomson one.

In order to account for the interference between the waves scattered by each electron in the atom the incoherent scattering function $S(x, Z)$ is introduced. It is a generalisation of the atomic form factor to include excited states.
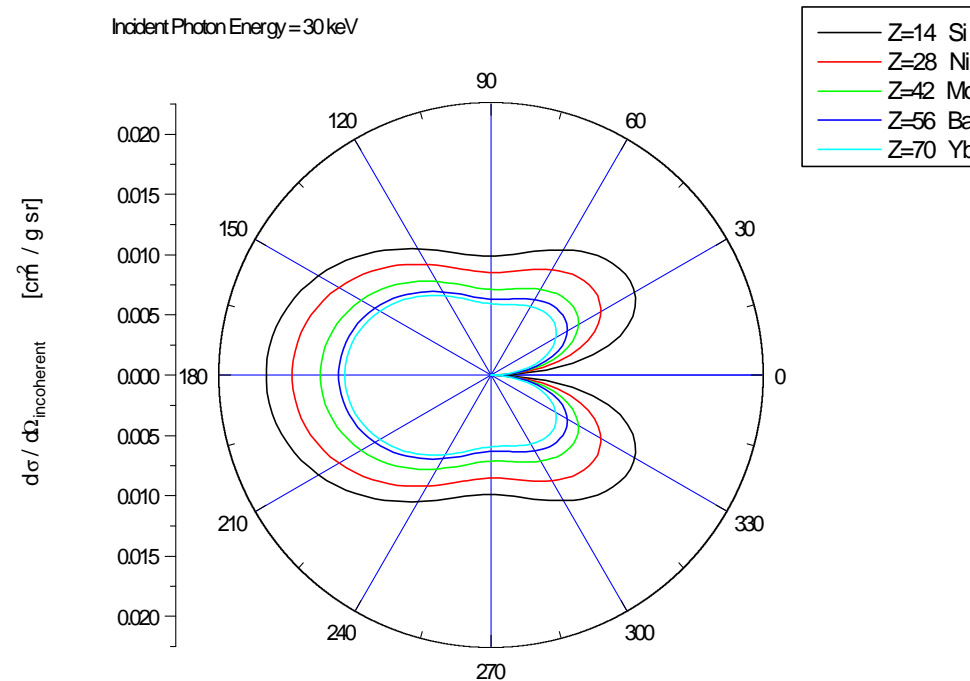
Indicating with ε the energy of an excited stationary state as measured from the ground level we can write

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

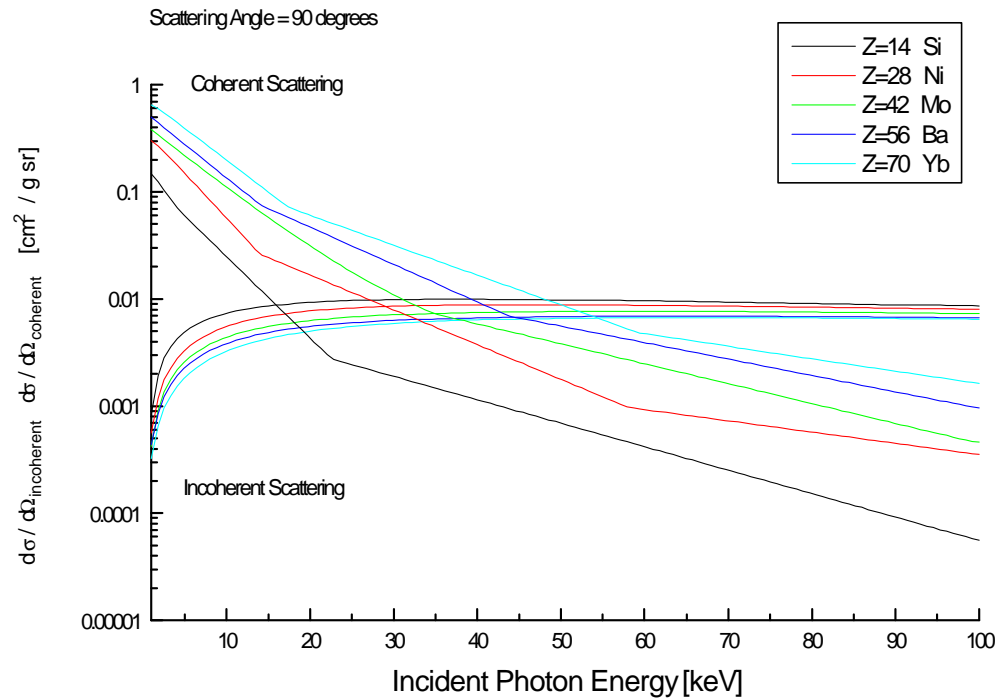The incoherent scattering function is then

$$S(q,Z) = \int_{e>0} |F_e(q,Z)|^2$$

Incident Photon Energy = 30 keV

Inelastic scattering differential cross section for different elements as a function of the scattering angle and for a fixed incident photon energy equal to 30 keV.

A comparison between the elastic and inelastic processes shows that the first ones are more important for small energies and high Z elements while for the upper part of the spectrum and the lighter elements the other ones become dominant.

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Scattering Angle = 90 degrees

Coherent Scattering

——	Z=14 Si
——	Z=28 Ni
——	Z=42 Mo
——	Z=56 Ba
——	Z=70 Yb

Incoherent Scattering

$d\sigma / d\Omega_{incoherent}$ $d\sigma / d\Omega_{coherent}$ [cm^2 / g sr]

Incident Photon Energy [keV]

Elastic and inelastic scattering differential cross section for different elements as a function of the incident photon energy for a fixed scattering angle equal to 90 degrees. (Calculated using the data from reference

The scattering coefficients $\sigma_{elastic}$ and $\sigma_{inelastic}$ which contribute to the total linear absorption coefficient are the total scattering cross sections, obtained by integration over the solid angle $d\Omega$.

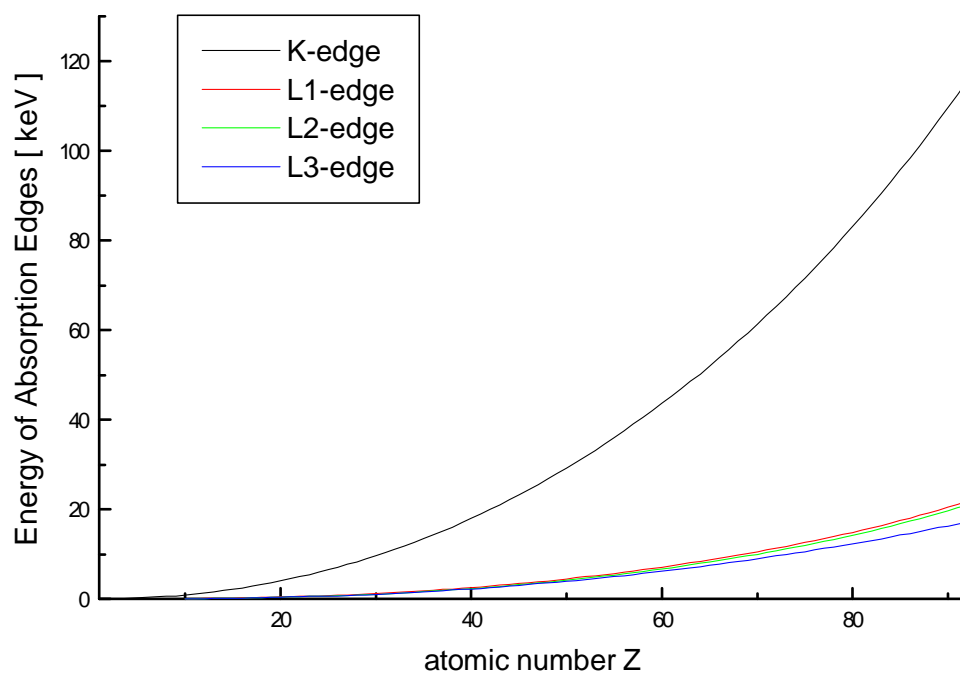$$\sigma_{el,in} = \int \frac{d\sigma_{el,in}}{d\Omega} d\Omega$$

They are therefore angle independent.

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Photoelectric absorption

It is the interaction which leads to the fluorescence photons. Fortunately it is dominant in the energy range we are interested in. A photon incident on an atom and having energy greater than the extraction potential of an electron in a certain shell may remove the electron and leave a vacancy.

The extraction potentials are also known as absorption edges. At this energy the photoelectric absorption coefficient τ presents a discontinuity.


Energy of photoelectric absorption edges versus atomic number of the elements.

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The total photoelectric absorption coefficient τ consists of the sum of the coefficients for the single shells.

When the photons reach an energy equal to an absorption edge, τ increases abruptly because the photons are suddenly able to remove some more electrons.

$$t = t_K + t_{L1} + t_{L2} + t_{L3} + t_{M1} + \ldots$$
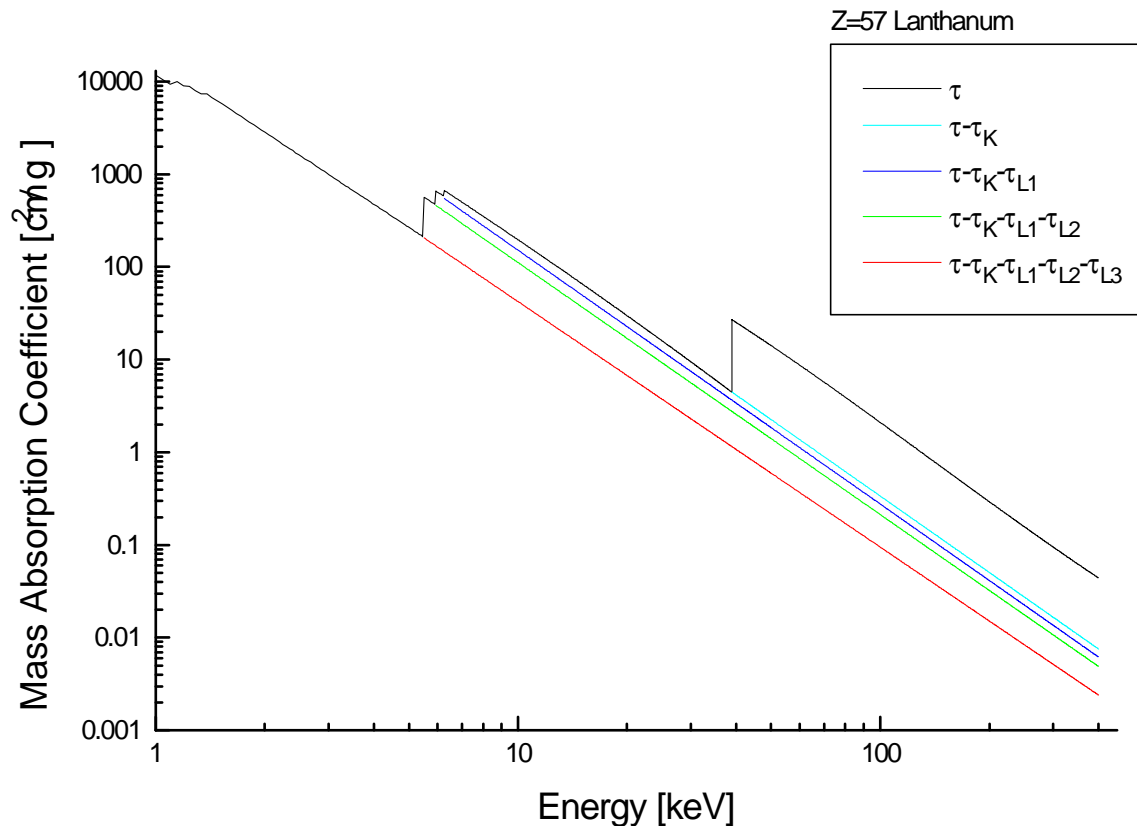
*Mass absorption coefficient of Lanthanum (Z=57)* versus *energy **of incident photons split in its components.***

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Between two absorption edges τ decreases with the photon energy approximately following Bragg-Pierce law

$$t_j = k_j \frac{Z^3}{E^{\frac{8}{3}}}$$

k is a constant which changes with the element and the shell.

At the edge energy the photoelectric absorption coefficient τ presents a discontinuity. Such discontinuity is described through the *jump ratio r*

The edge discontinuity is described through the *jump ratio r*
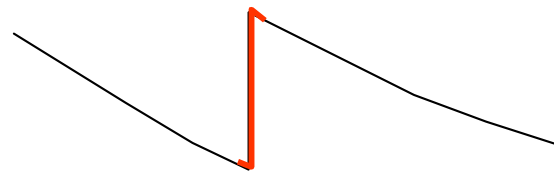
$$r = \frac{\lim_{E \to edge^+} t(E)}{\lim_{E \to edge^-} t(E)}$$

One of the components of the single shell photoelectric absorption coefficient may be calculated from τ if the jump ratios are known. At an energy above the *k*-edge we have:
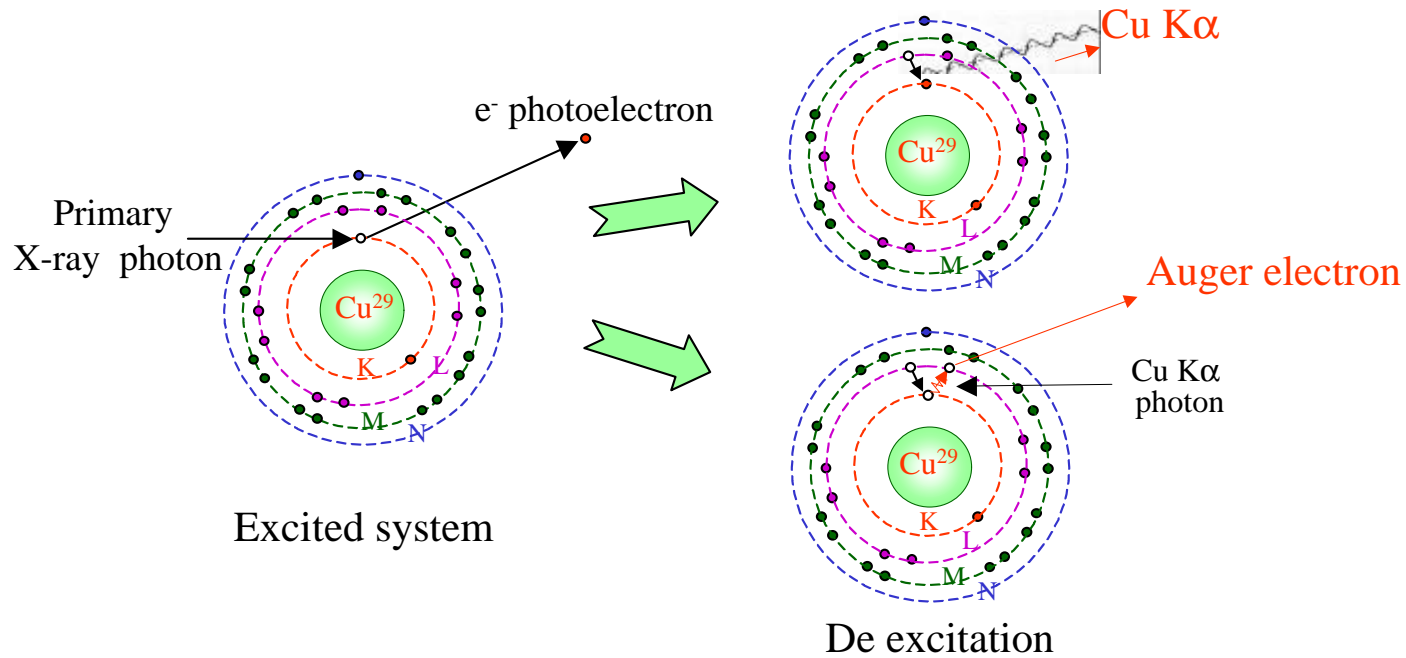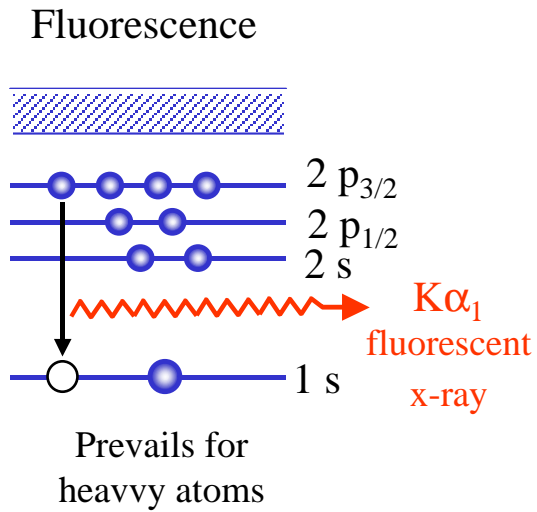
$$t_K = t \frac{(r-1)}{r}$$

De-excitation mechanisms

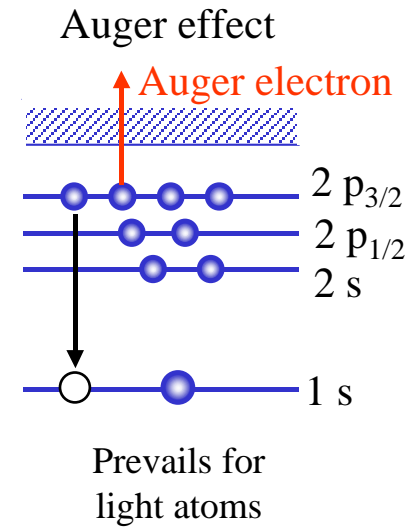Competing decay processes following the presence of a core hole

| Radiative transition: Fluorescence | Non radiative transition: Auger effect |

Excited system

De excitation

Fluorescence

2 $p_{3/2}$
2 $p_{1/2}$
2 s

$K\alpha_1$
fluorescent
x-ray

1 s

Prevails for
heavvy atoms

X_s = probability of emission
of a fluorescence photon;
s denotes the edge.

Auger effect

Auger electron

2 $p_{3/2}$
2 $p_{1/2}$
2 s

1 s

Prevails for
light atoms

A_s = probability of emission
of a fluorescence photon from an s edge.

Fluorescence yield: $w_s = \dfrac{X_s}{X_s + A_s}$

Auger yield: $1 - w_s$

W_s

Fluorescent Yield

K

L

Atomic Number Z
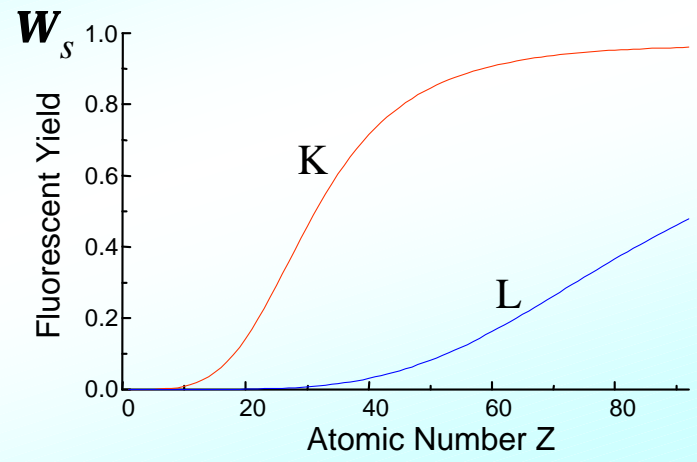
Because of Auger effect the lines of a givel series (for instance the K lines: $K_{\alpha 1}$, $K_{\alpha 2}$, $K_{\beta 1}$, …) are not as intense as the would be predicted from the number of vacancies which are present at the associated energy level (tke k level for the K lines).

The K fluorescence yield is defined also as the number of photons of all K lines emitted in the unit time divide by the number of K vacancies formed in the same time, i.e.;

$$w_K = \frac{n_{K_{a1}} + n_{K_{a2}} + n_{K_{b1}} + \dots}{N_K}$$

$\left(n_K \right)_i$ Represets the number of photons of the spectral line i emipptted in unit time

N_K is the rate of production of vacancies in the K shell

The fluorescence yields characteristic of the the shell L, ω_L or the shell M, ω_M,… are defined similarly.

Were it not for the Auger effect the yield fluorescence of a given line series would always be 1.

The fluorescent yield depends on the atomic number Z and the line series; an empirical approximation is given by:

$$w = \frac{Z^4}{A + Z^4}$$

Where A is a constant having value 10^4 for K lines and 10^8 for L lines.

The Auger yield is defined as the ratio of the Auger electrons prosuced in the unit time and the vacancies created in the same time interval.
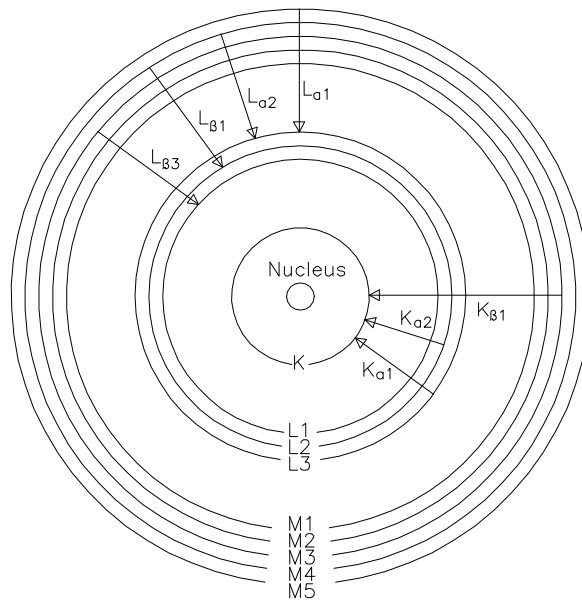
The Auger Effect

The Auger effect, and the fluorescence photons are secondary interactions: they can only happen after a photoelectric absorption has occurred.
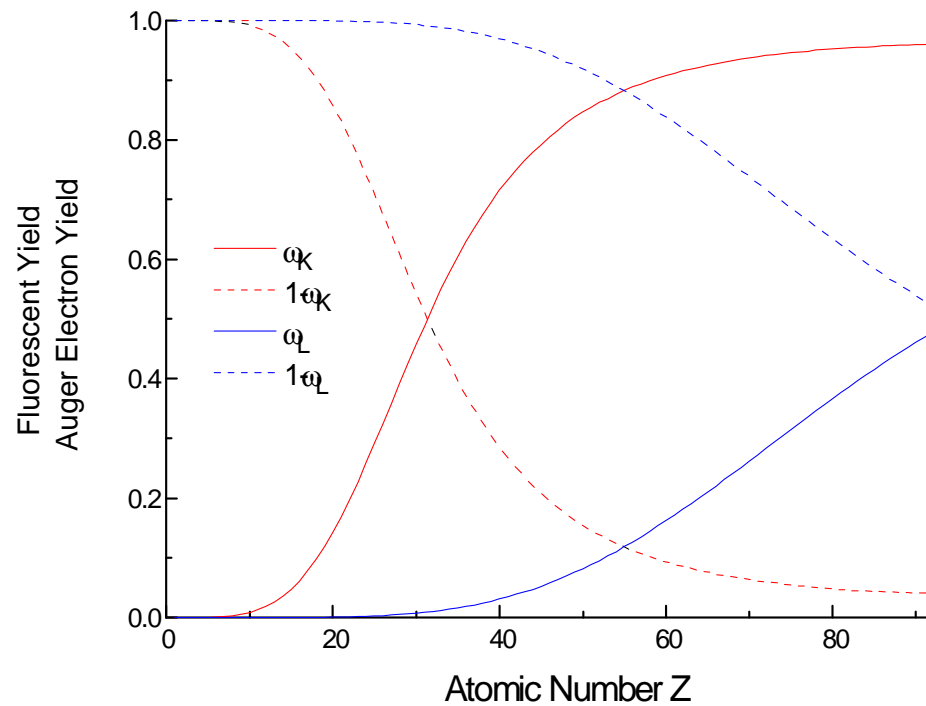
Fluorescent yield and Auger electron yield versus atomic number of the elements. (Curves calculated using fit parameters from reference

The characteristic spectrum

It sets the basis for elemental fluorescence analysis.
It consists of a series of discrete energies corresponding
to the energy difference between two atomic levels
and is therefore characteristic of the emitting element.

When a K-shell electron is removed the vacancy can be
filled by an L-electron, this will result in another vacancy
and photons belonging to different lines will be emitted.
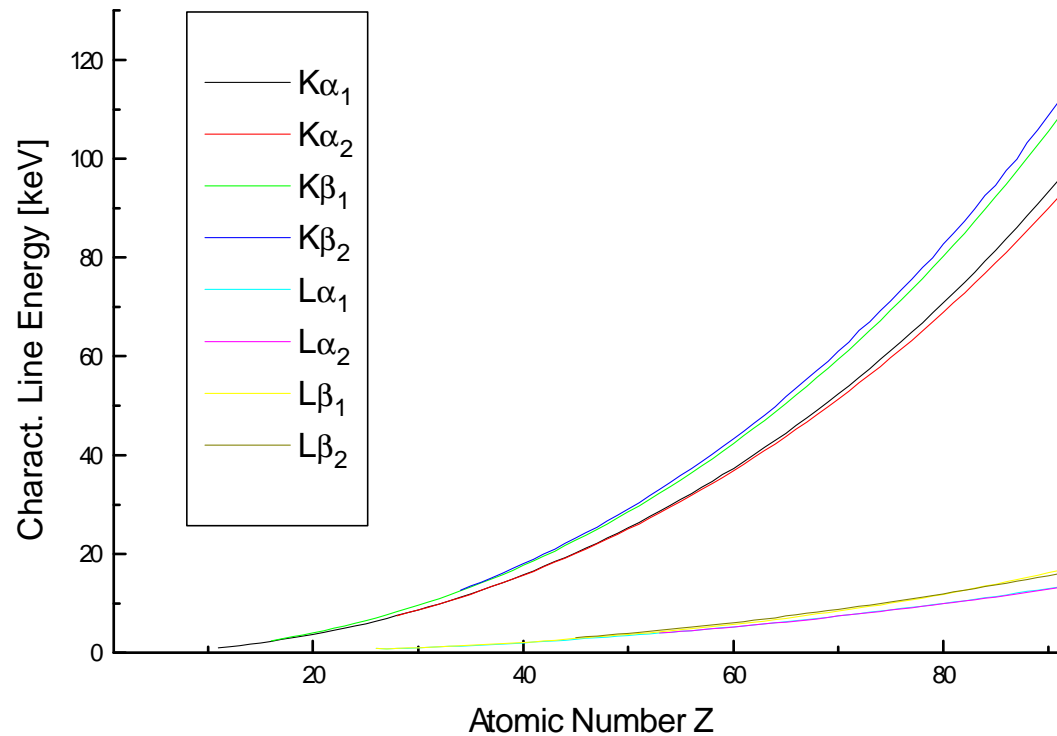
$$D_n \, {}^1 \, 0$$

$$D_l = \pm 1$$

$$D_j \, {}^1 \, \pm 1, \, 0$$

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

Moseley was the first to investigate and find the relationship between the atomic number of an element and the energy of its spectral lines and it can be described as

$$E (Z) = k_j (Z - s_j)^2$$

where k_j and s_j are fixed for a certain transition j

Energy of the most important lines versus atomic number Z.

The atomic scattering factors.

In the classical theory of dispersion the atom is assumed to scatter radiation as if it was formed by dipole oscillators whose natural frequencies are those of the absorption edges of the electronic shells. In this approximation oscillators are formed by bound electrons moving harmonically with respect to a fixed nucleus. An electromagnetic wave falling on an atom forces the electrons to oscillate; the dipole radiates with same frequency of the incident wave. The dipole scattering factor is defined as the ratio of the amplitude of the wave scattered by a bound electron to the one scattered by a free electron.
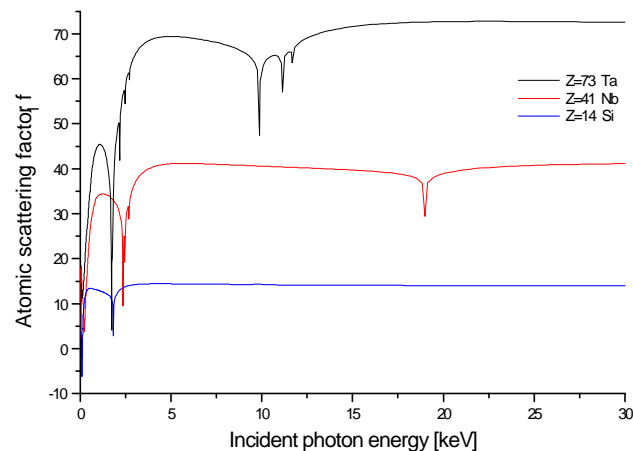
$$f = \frac{A_{bound}}{A_{free}}$$

The quantity obtained happens to be complex and is usually separated in its components.
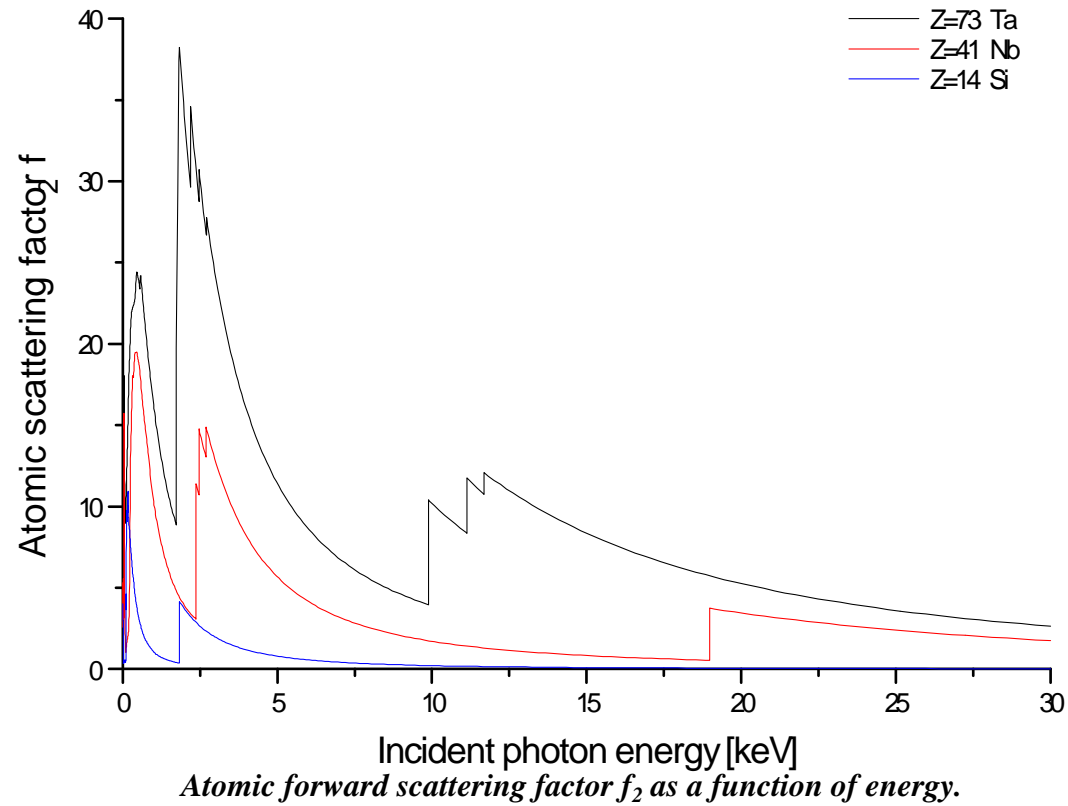
$$f = f' + if''$$

The expression is generalised by summing the contributions of all the oscillators contained in the atom and we can write

$$f = f_1 + if_2$$

Atomic forward scattering factor f₁ as a function of energy

Atomic forward scattering factor f_2 as a function of energy.

The real part of the atomic scattering factor for energies above and far away from the absorption edge is approximate equal to the number of "relevant" electrons: for a photon energy above the K absorption edge $f_1=Z$ for, an energy betwee the L3 and the K absorption edge $f_1=Z-2$ and so on.

It can then be shown that the refractive index for a material with N atoms per unit volume is given by

$$n = 1 - \frac{N\,r_0\,\lambda^2}{2\pi}\left(f_1 + if_2\right)$$

in which $N = \dfrac{N_a\,\rho}{A}$ is the number of atoms per unit volume

and
e is the electron charge
c is the velocity of light
m_0 is the electron rest mass

$$\delta = \frac{N_a r_0}{2\pi}\frac{\rho}{A}\lambda^2 f_1 \qquad\qquad \beta = \frac{N_a r_0}{2\pi}\frac{\rho}{A}\lambda^2 f_2$$

Material	density ρ [g/cm^3]	$\delta\cdot10^{-6}$	$\beta\cdot10^{-8}$
Plexiglas	1.16	0.9	0.055
Glassy carbon	1.41	1.0	0.049
Quartz glass	2.20	1.5	0.46
Silicon	2.33	1.6	0.84
Tantalum	16.6	9.1	87.5
Platinum	21.45	11.7	138.2
Gold	19.3	10.5	129.5

*Real and imaginary part of the refractive index calculated for Mo $K\alpha$ radiation (**17.478** keV)*

Reflection and refraction of x-rays

Reflection and refraction of x-rays can be described with the same formalism as for visible light. A monoenergetic beam meeting the border surface between two media with different dielectric constant ε is considered. The incident, reflected and refracted beam are approximated to plane waves. On the border surface the contour conditions derived from Maxwell laws (Fresnel conditions) are applied and an analytical form for the reflected and for the refracted beam is obtained.
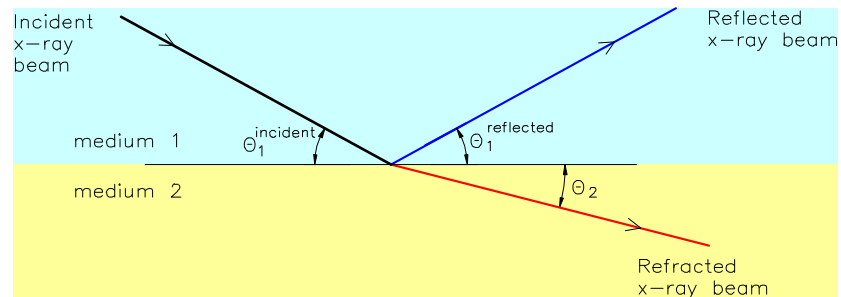
Reflection and refraction of x-rays on the border surface between two media

A first consequence of the Fresnel conditions is that the frequency of the outgoing beams equal the frequency of the incoming beam. Moreover the incident angle is equal to the reflection angle

$$\boldsymbol{q}_1^{\,incident} = \boldsymbol{q}_1^{\,reflected}$$

and the refraction angle follows Snell's law.

$$\frac{n_1}{n_2} = \frac{cos\,\theta_2}{cos\,\theta_1}$$

n is called the refractive index and is defined by

$$n = \frac{c}{v}$$

where c is the velocity of light in vacuum and v is the phase velocity of light in a medium.
The phase velocity in a medium is energy dependent and is in the x-ray region bigger than c; as a
consequence the refraction index also depends on the energy of the incident photon and it is for x-rays
slightly smaller than 1. Usually absorption effects in the media cannot be avoided and the index is a
complex number. Thus it is written as

$$n = 1 - \boldsymbol{d} - i\boldsymbol{b}$$

The coefficient δ is called decrement because it reduces the real part of the refractive index from the
unitary value. The coefficients β is a measure of the absorption and is related to the linear photoelectric
absorption coefficient by

$$\boldsymbol{b} = \frac{\boldsymbol{l\,m}}{4\boldsymbol{p}}$$

Critical angle and total reflection

The refractive index for air can be approximated to the refractive index of vacuum which is 1.
Snell's law becomes hence

$$\frac{1}{n_2} = \frac{\cos q_2}{\cos q_1}$$

n_2 is smaller than 1. This means that the refractive angle θ_2 must be smaller than the incident angle θ_1.
The incident angle for which the refraction angle becomes 0 is called the critical angle
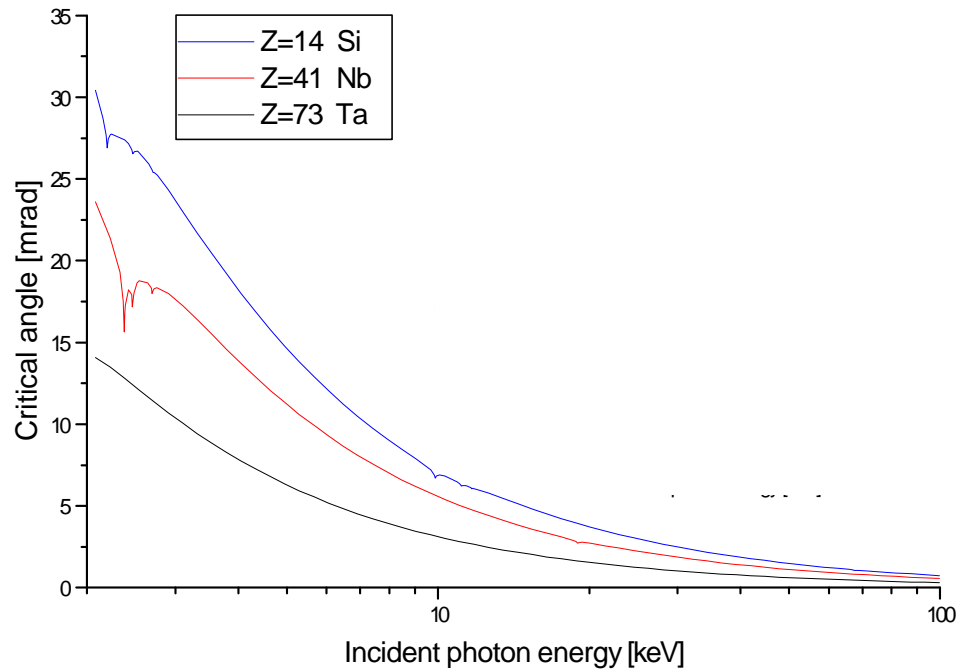
$$\cos q_{crit} = n_2$$

Since n_2 is very close to one θ_{crit} must be very close to 0 and the cosine can be approximated with the first two terms of the Taylor series in 0.

$$\cos q_{crit} \approx 1 - \frac{q_{crit}^2}{2} \approx n_2$$

If we ignore the imaginary component of the refractive index we obtain

$$q_{crit} \approx \sqrt{2d}$$

Theoretical critical angle for different reflector materials as a function of incident photon energy in a linear -logarithmic graph and log-log graph. Far away from the absorption edges the ratio between the critical angle for different materials is constant.

Material	critical angle [mrad]		
	17,5keV	60keV	100keV
Silicon	1.8	0.5	0.3
Niobium	3.1	0.9	0.6
Tantalum	4.2	1.2	0.7
Platinum	4.8	1.4	0.8
Gold	4.5	1.3	0.8

Theoretical critical angle for different materials and different energies of the incident photons.

Reflectivity

The reflectivity of a surface is defined as the ratio

$$R = \left| \frac{\vec{E}_{incident}}{\vec{E}_{reflected}} \right|^2$$

where

$\vec{E}_{incident}$ is the electric field associated to the incident beam

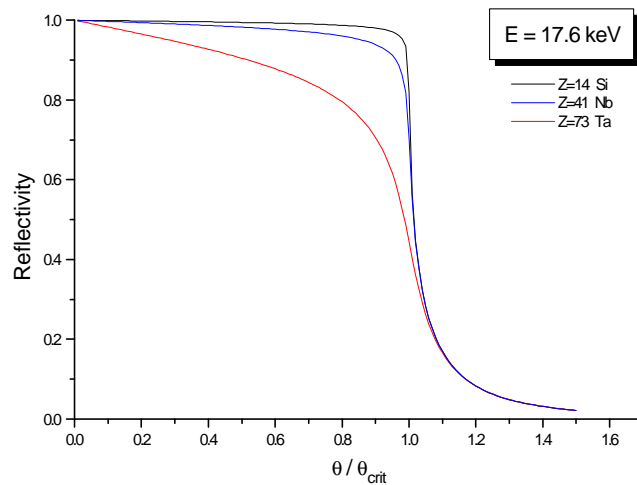$\vec{E}_{reflected}$ is the electric field associated to the reflected beam

Using Fresnel formulas we get

$$R = \frac{h - \sqrt{2} \, \dfrac{\boldsymbol{q}}{\boldsymbol{q}_c}(h-1)^{\frac{1}{2}}}{h + \sqrt{2} \, \dfrac{\boldsymbol{q}}{\boldsymbol{q}_c}(h-1)^{\frac{1}{2}}}$$
in which
$$h = \left(\frac{\boldsymbol{q}}{\boldsymbol{q}_c}\right)^2 + \left\{ \left[\left(\frac{\boldsymbol{q}}{\boldsymbol{q}_c}\right)^2 - 1 \right]^2 + \left(\frac{\boldsymbol{b}}{\boldsymbol{d}}\right)^2 \right\}^{\frac{1}{2}}$$

E = 17.6 keV

Z=14 Si
Z=41 Nb
Z=73 Ta

Theoretical reflectivity different materials as a function of the ratio $\boldsymbol{q}/\boldsymbol{q}_c$ for a fixed incident photon energy.

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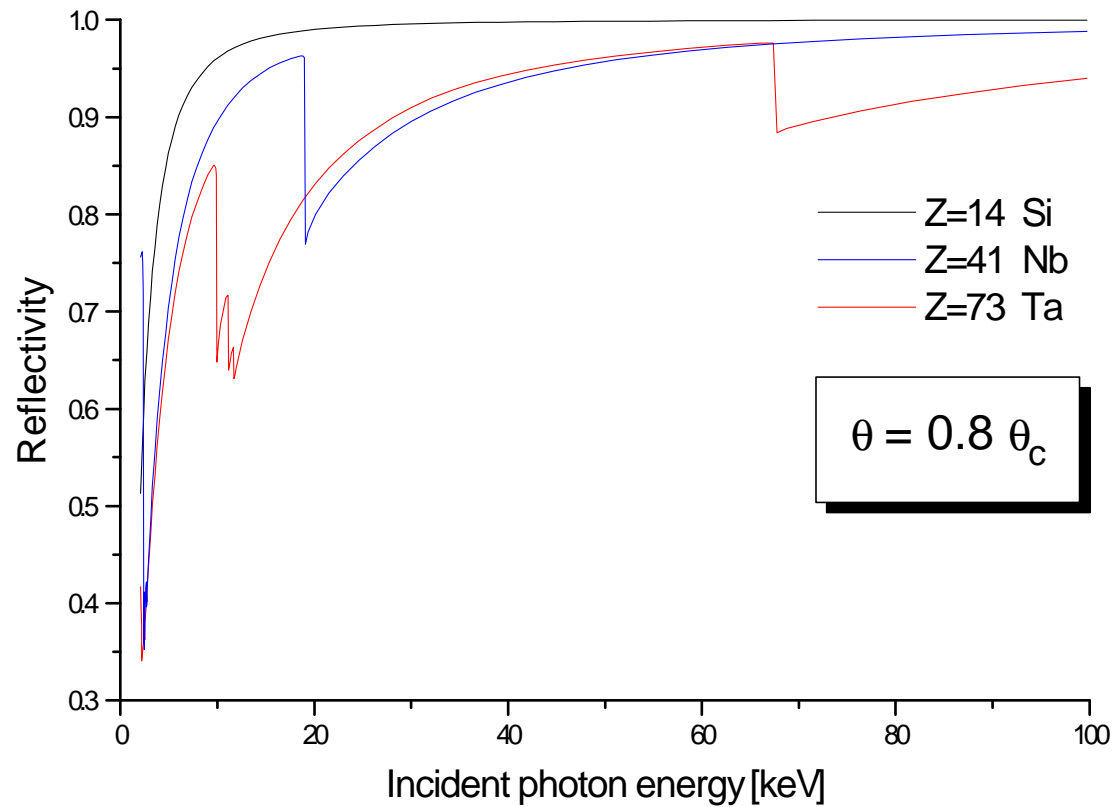
*Theoretical reflectivity for different reflector materials as a function of incident photon energy at a fixed ratio **q/q**c.*
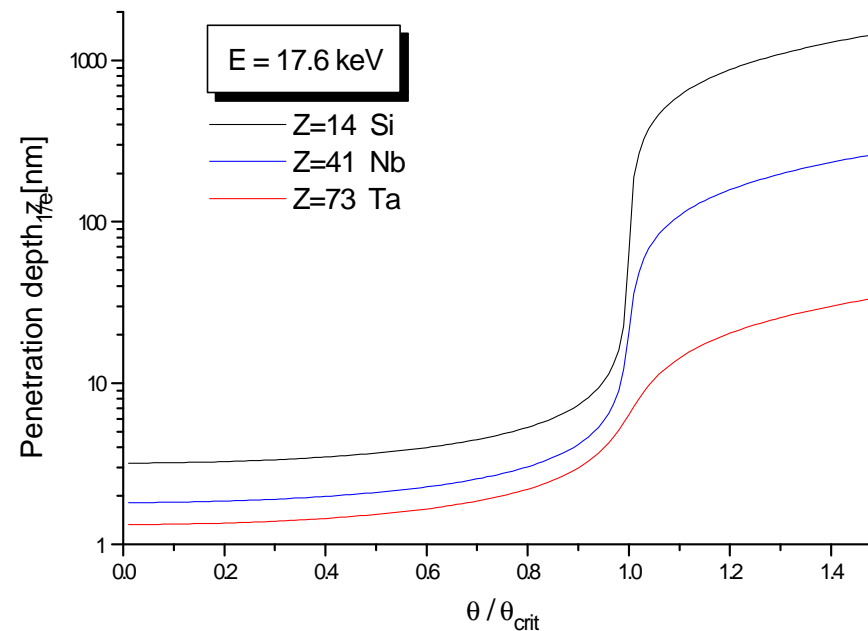
For the calculation it is assumed that the reflecting surface is „perfectly" polished for every material.

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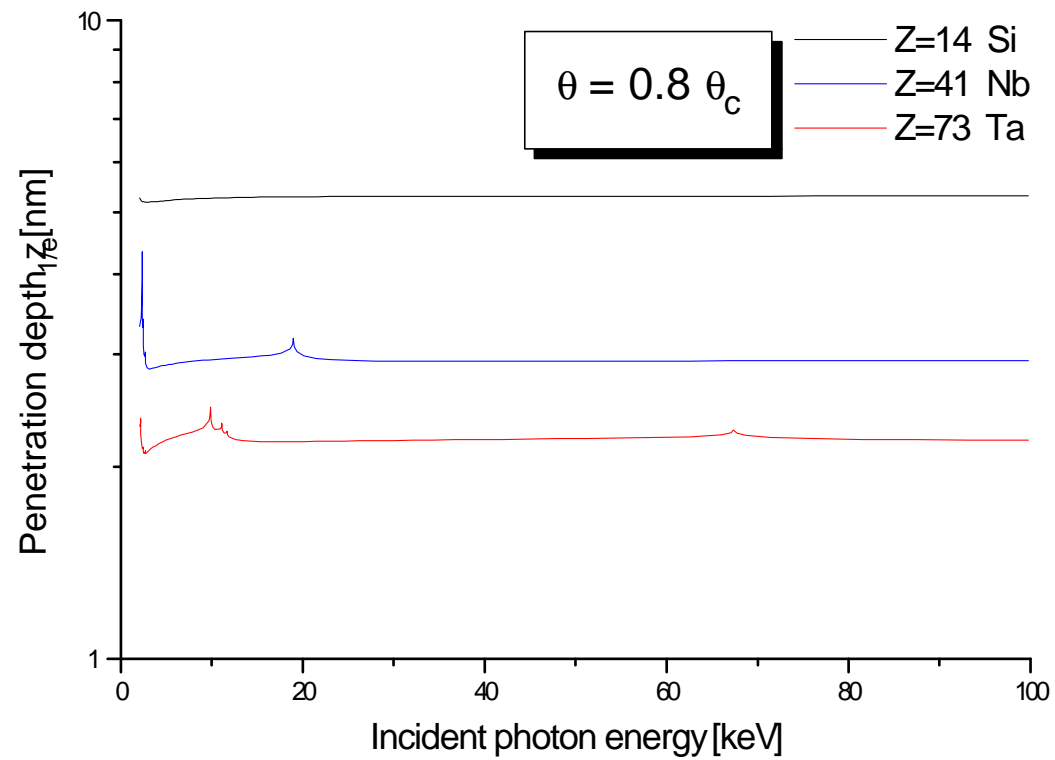
Penetration Depth.

When a beam coming from vacuum or air hits the surface of an optically denser medium under an angle smaller than the critical one it is „totally" reflected. This reflection does not entirely occur in the first layer of atoms but the beam penetrates into the material and the importance of the phenomenon depends on the reflector material; from the theoretical considerations already explained it can be quantified. With $z_{1/e}$ is indicated the depth at which the beam intensity is reduced of a factor 1/e

$$z_{1/e} = \frac{\mathbf{h}c}{2E} \frac{\sqrt{2}}{\left\{\left[\left(\mathbf{q}^2 - \mathbf{q}_c^2\right)^2 + 4\mathbf{b}^2\right]^{\frac{1}{2}} - \left(\mathbf{q}^2 - \mathbf{q}_c^2\right)\right\}^{\frac{1}{2}}}$$

*Theoretical penetration depth for different reflector materials as a function of the ratio **q/q**c for a fixed incident photon energy.*

Giuseppe Dalba, *La Fisica dei Raggi X,* Dipartimento di Fisica, Università di Trento, a.a. 1999-2000

Theoretical penetration depth for different reflector materials as a function of incident photon energy at a fixed ratio q/q_c

For the light elements the penetration depth increases, for these elements and for high energies inelastic scattering becomes important and therefore the background „noise" grows up.

Diffraction

An x-ray beam impinging on an ordered, periodical structure like a crystal or a multilayer undergoes multiple reflections from the different planes of the lattice or the delimitation surfaces between the various layers.
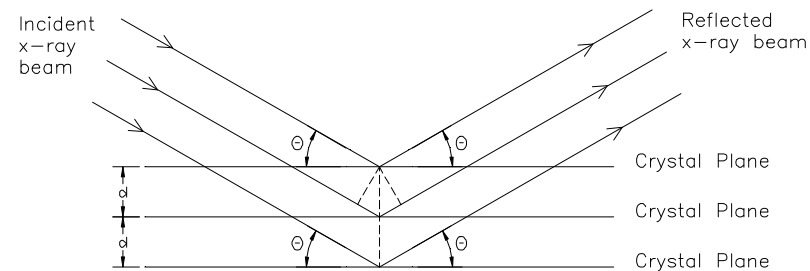
Multiple reflection of an x-ray beam from the different plane s of a crystal.

The reflected waves interfere with each other and diffraction patterns are obtained. In first approximation (that is if we ignore dispersion effects inside the crystal) the phenomenon follows Bragg's law

$$n\lambda = 2d \sin\theta$$

where n is the order diffraction, d is the interplanar spacing and θ is the angle between the reflecting planes and the incident beam.