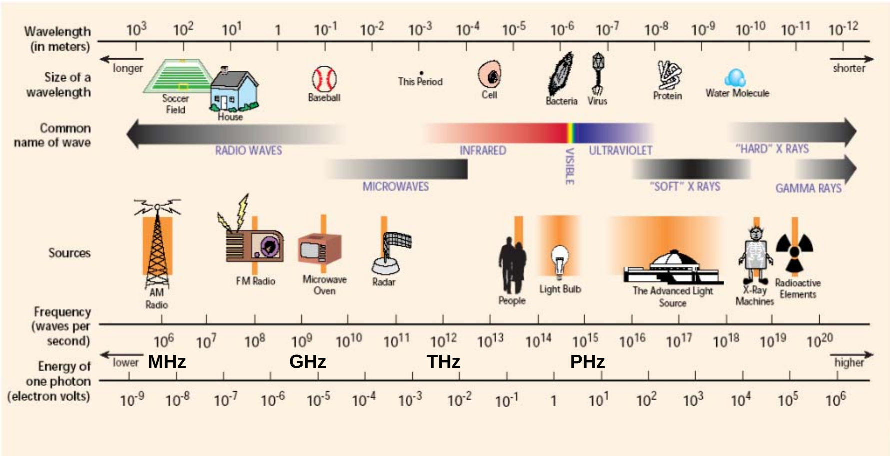
2. Interaction with Matter
The Basics

What you will learn about…

- Basic Equations
- Overview of Techniques
- X-ray Scattering Processes:
  - Compton Scattering
  - Thomson Scattering
  - Photoelectric Absorption
- Atomic Scattering Factors
- Refractive Index
- Refraction and Reflection
- Absorption
- X-ray Fluorescence vs. Auger Emission
- Coherence

The Electromagnetic Spectrum



http://www.lbl.gov

Basic Equations

Energy of a photon?

ν & λ = radiation frequency (Hz) & wavelength (m)

To determine the wavelength of photons for a given photon energy:

➔

So 1 Å x-ray photon has an energy of 12.398 keV

Visible light: __________, X-rays:______________

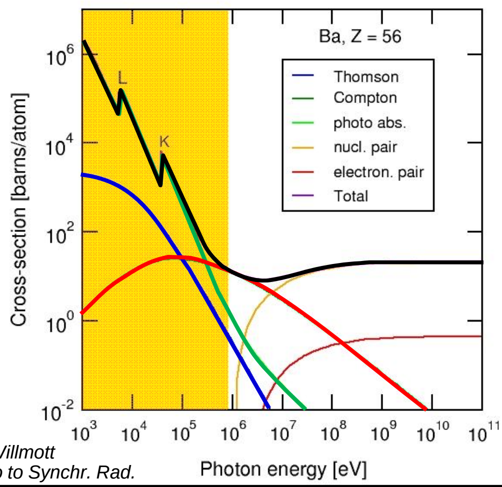
Wavenumber: ___________

➔Spatial frequency:
number of wavelengths per 2π units of distance

X-ray Scattering Processes

X-ray Scattering Processes

- Cross-sections for various processes involving interaction of x-rays with matter - primary scatterer is the **electron**
- Plot for Ba; orange area highlights upper energy range covered by synchrotron sources



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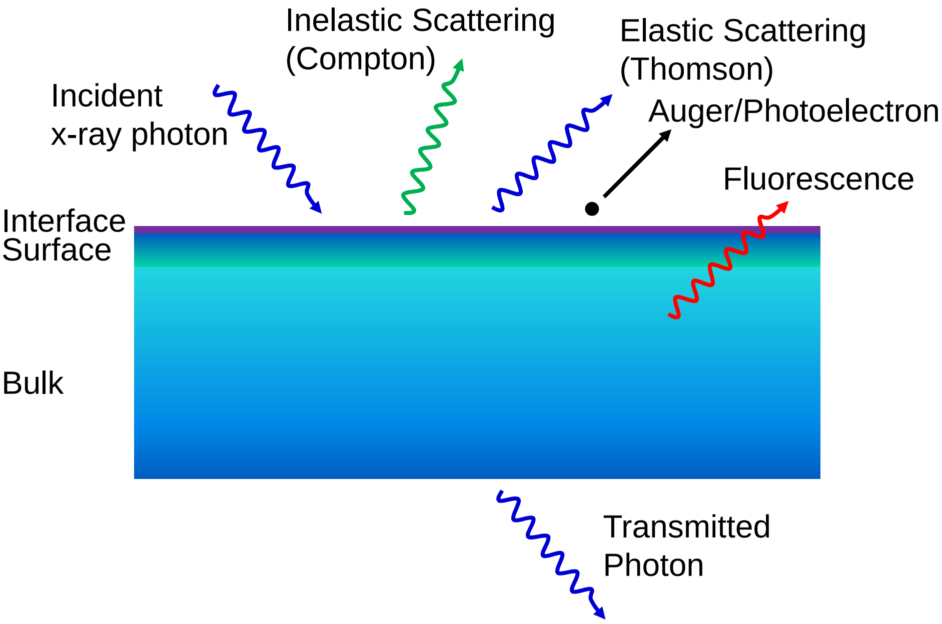
Key scattering processes:

- **Photoelectric Absorption**
- **Thomson Scattering (elastic)**
- **Compton Scattering (inelastic)**

➔ **Total !**

1 barn = 10^{-24} cm^2
= 10^{-28} m^2

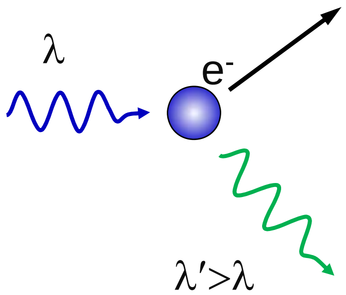
Key Phenomena



Compton Scattering

Inelastic Scattering

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



Compton scattering length:
λ of a photon whose energy is the same as the rest-mass energy of the electron

So equate mc^2 with hc/λ:

$$\frac{h}{m_e c} = 2.43 \text{ x } 10^{-2} \text{ Å}$$

Thomson Scattering

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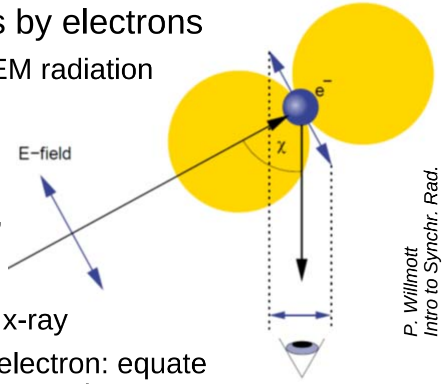
Elastic scattering of photons by electrons

- Electron oscillates with E-field of EM radiation
- Re-emits at same frequency
- Seen intensity ____________
- Intensity distribution → "Electromagnetic Dipole radiation"
- **Thomson scattering length:**
  - Ability of electron to scatter an x-ray
  - Simply classical radius of free electron: equate rest mass energy mc^2 with electrostatic energy i.e. Coulomb energy at a distance r from a point charge $\frac{e^2}{4\pi\varepsilon_0 r_0}$ to give:



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- Elastic scattering amplitude ∝ r_0 and Z

Atomic Scattering Factors

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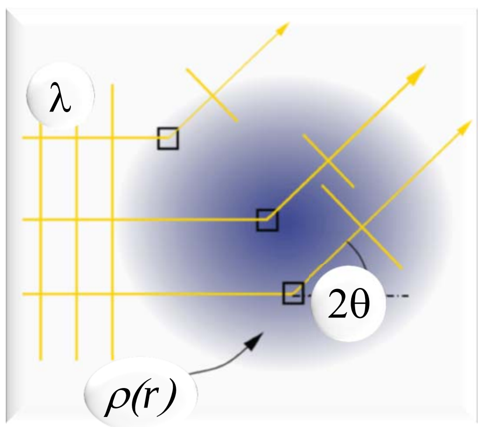
Atomic scattering factor:
"measure of the scattering amplitude of a wave by an isolated atom



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Atomic Scattering Factor

The scattering amplitude $f(\boldsymbol{Q})$ from an atom (containing Z electrons) at an angle 2θ relative to incoming beam:

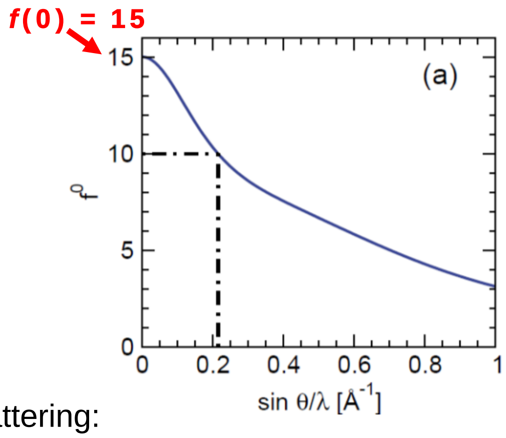
$$f(\boldsymbol{Q}) = \int_{\text{atom}} \rho(\boldsymbol{r}) \cos(\underbrace{\boldsymbol{Q} \cdot \boldsymbol{r}}_{\phi})\, d\boldsymbol{r}$$

Or, more compactly for distributions with spherical symmetry:

$$f(\boldsymbol{Q}) = \int_{\text{atom}} \underbrace{e^{i\boldsymbol{Q}\cdot\boldsymbol{r}}}_{\text{Phase Factor}} \underbrace{\rho(\boldsymbol{r})}_{\text{Electron Density}}\, d\boldsymbol{r}$$

Atomic Scattering Factor

Atomic scattering factor as a function of Bragg angle for a given λ. Example for phosphorus (Z = 15):



Forward scattering:

- $2\theta = 0$; $\boldsymbol{Q} = 0$; $\phi = 0$
- $f(0) = Z$, i.e. the number of electrons in the atom!

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Atomic Scattering Factor

Things you should know:

Atomic scattering factor describes the:
"total scattering amplitude of an atom as a function of sinθ/λ"

- Also called "atomic form factor"
- Proportional to $\boldsymbol{Q}$, the scattering vector
- Consider electron cloud around nucleus - not a point scatterer!
- Expressed in units of scattering amplitude produced by one electron
- f(sinθ/λ) = f(0) = Z, the atomic number

Refractive Index

Index of refraction n at a wavelength λ

→ Response of electrons in matter to electromagnetic radiation

→ In x-ray regime is related to the atomic scattering factors of the individual atoms in a material

$$n = 1 - \delta - i\beta = 1 - \frac{r_0}{2\pi}\lambda^2 \sum_i N_i \underbrace{f_i(0)}_{f_1 + i f_2}$$

Refractive index Decrement (δ)
Refraction & Reflection

Absorption Index (β)
Absorption

…so n has a real and imaginary part $n = n_R + in_I$

Magnitude of δ

Refraction & Reflection

$$\delta = \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_{1i}(0)$$

electron density

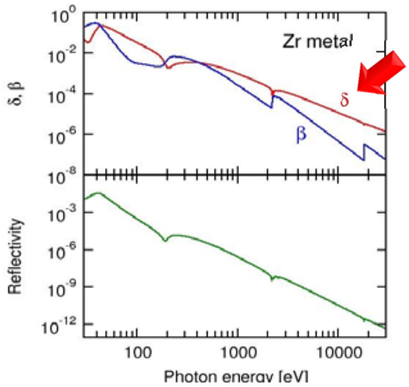
For $\lambda \sim 1$ Å

$\frac{r_0}{2\pi}\lambda^2 = 4.5 \times 10^{-6}$ Å^3

Typically $\rho \sim 1$ e/Å^3

Therefore $\delta \sim 10^{-5}$

Note: $\delta \propto \lambda^2 \propto E^{-2}$



Magnitude of β

Absorption

$$\beta = \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_{2i}(0)$$

~ electron density * 0.01

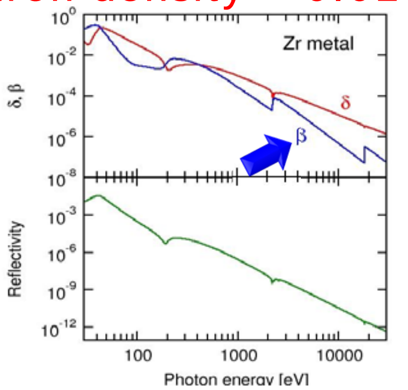
For $\lambda \sim 1$ Å

$\frac{r_0}{2\pi}\lambda^2 = 4.5 \times 10^{-6}$ Å^3

Typically $\beta \sim 10^{-8} - 10^{-7}$

With $\beta \propto E^{-4}$

$\beta \sim$ 2 orders of magnitude smaller than δ



Refraction and Reflection

Ignoring β

$$n = 1 - \delta$$

$$\delta = \frac{r_0}{2\pi}\lambda^2 \sum_i N_i f_{1i}(0)$$

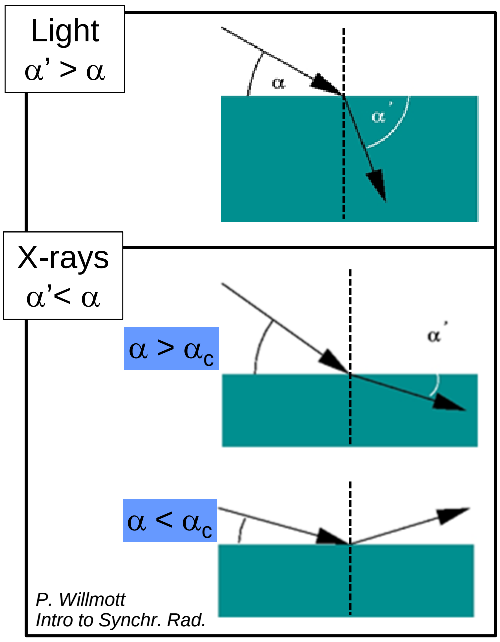
$\sim 10^{-5}$

Refraction of light by transparent medium >1

Refractive index for x-rays is just < 1

Snell's Law:

$$\frac{\cos\alpha}{\cos\alpha'} = n$$



Refraction and Snell's Law

$$\frac{\cos\alpha}{\cos\alpha'} = n$$

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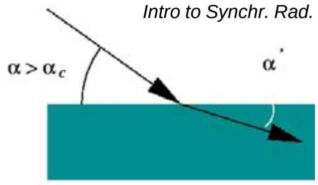
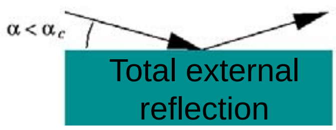


Critical angle ($\alpha' = 0$) is minimum angle for which x-rays refracted into bulk of material:

$\cos\alpha_c = n = 1 - \delta$

For small angles:

$$\cos\theta \approx 1 - \frac{\theta^2}{2}$$



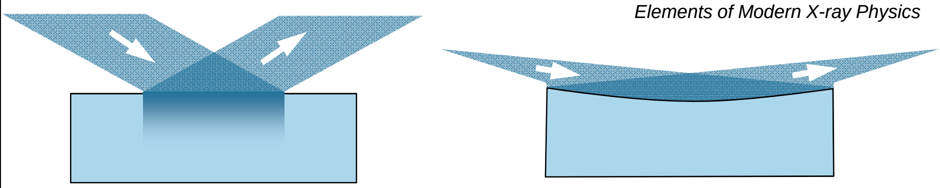
So, $\delta \approx \frac{\alpha_c^2}{2} \rightarrow \alpha_c = \sqrt{2\delta} \sim 3 \times 10^{-3}$ radians (0.15°)

N.B. $\delta \propto 1/E^2 \Rightarrow \alpha_c \propto 1/E$

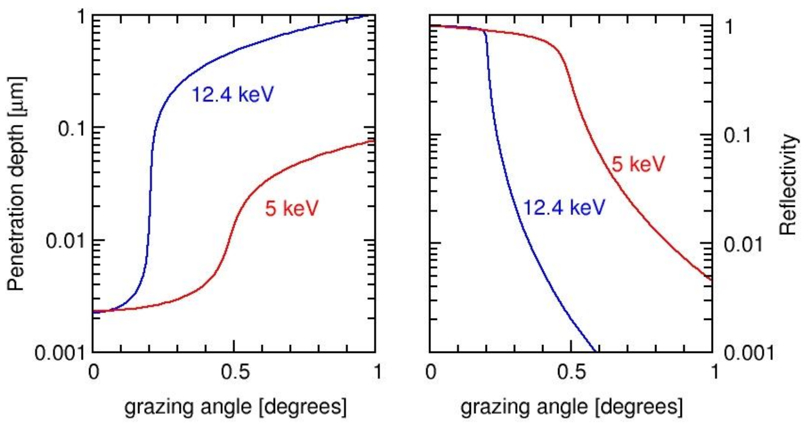
So at low incident angles, x-rays reflect from surfaces……

Evanescent Wave

After J. Als-Nielsen & D. McMorrow
Elements of Modern X-ray Physics



Evanescent Wave



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Absorption

Consider a plane electromagnetic wave

– In vacuum, wave function given by:

$$E(z,t) = E_0 \exp[i(\omega t - k_0 z)]$$

– In matter, with refractive index *n:*

$$E(z,t) = E_0 \exp[i(\omega t - n k_0 z)]$$

But since

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

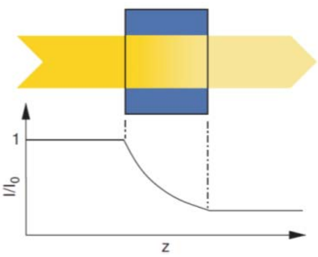
We obtain:

$$E(z,t) = E_0 \exp(-\beta k_0 z) \exp[i(\omega t - (1-\delta) k_0 z)]$$

Absorption

Listen!

$$E(z,t) = E_0 \underbrace{\exp(-\beta k_0 z)}_{\text{Attenuation of amplitude}} \underbrace{\exp[i(\omega t - (1-\delta) k_0 z)]}_{\text{Wave propagating in medium}}$$



intensity ~ amplitude^2

…so attenuation of intensity $e^{-2\beta k_0 z}$

Beer-Lambert equation $\frac{I}{I_0} = e^{-\mu z}$

Therefore the absorption coefficient $\mu = 2k_0\beta$

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Absorption

Therefore the absorption coefficient $\mu = 2nIk_0$

- reciprocal of the thickness of material which is needed to reduce the intensity of an electromagnetic wave by a factor of $1/e$
- Indication of electron density and electron binding energy, so sensitivity to different allotropic forms with different densities e.g. carbon, diamond, graphite, C_{60}
- But compounds that contain the same number of electrons per formula unit and have similar mass densities will have similar absorption properties except at absorption edges e.g. NaCl, MgS, AlP and Si where average number of electrons per atom is 14
- Therefore better to consider the atomic absorption cross-section of element σ_a, where $\mu = \rho_a \sigma_a = (\frac{\rho_m N_A}{A})\sigma_a$

Absorption

Atomic absorption cross-section of element σ_a, where

$$\mu = \rho_a \sigma_a = (\frac{\rho_m N_A}{A})\sigma_a$$

Absorption Coefficient (μ)

Atomic number density (ρ_a)

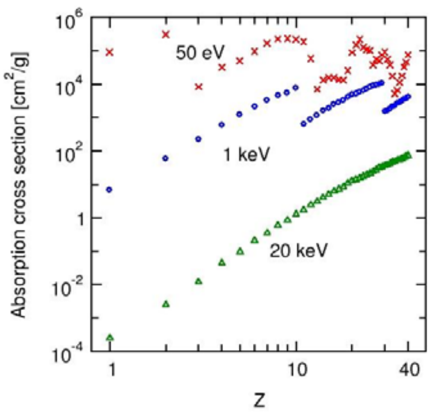
Mass density X Avogadro's Number / Atomic mass ($\frac{\rho_m N_A}{A}$)

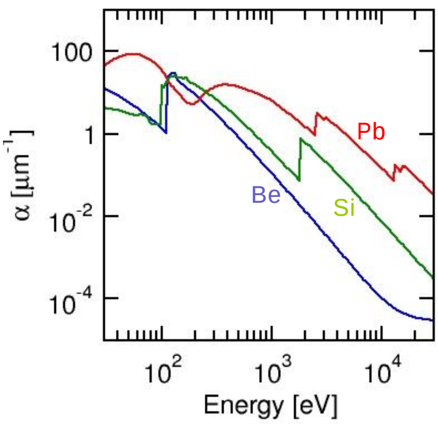
More commonly 'mass absorption coefficient':

$$\sigma_a\,[\mathrm{cm^2/g}] = \frac{N_A}{A}\sigma_a\,[\mathrm{cm^2}] = \frac{\mu}{\rho_m}$$

Absorption

- Strongly dependent on atomic number, approx. α Z^4
- Decreases with increasing photon energy approx. α E^{-3}

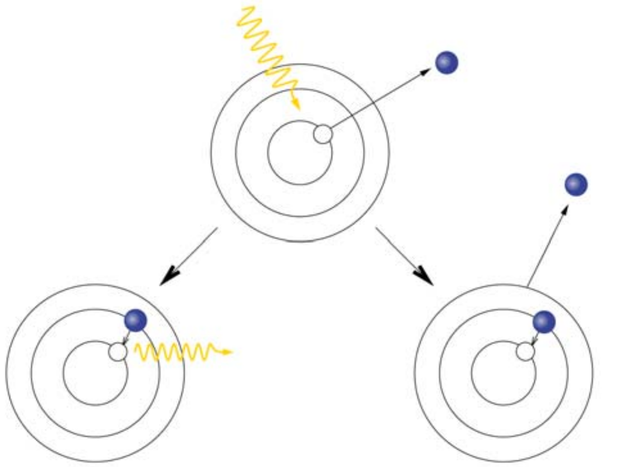




$\mu \propto Z^4$ $\mu \propto E^{-3}$

X-ray Fluorescence & Auger Emission

Two dominant processes following absorption of an x-ray photon and ejection of an x-ray photoelectron:



X-ray Fluorescence (XRF) Auger electron emission

X-ray Fluorescence - Notation

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Barkla assigned letters, starting at K in case there might be a more energetic series:

K, L, M….: $n = 1, 2, 3\ldots$

Relaxation of an electron to the K-shell → K x-rays

Relaxation of an electron to the L-shell → L x-rays….

Suffixes, greek

α, β ....: Electron drops from L-shell, M-shell etc.

At least for K shell…see next slide!

Suffixes, number

1: from l + 1/2

2: from l - 1/2

Where l is the shell from which the electron drops

e.g. $K_{\alpha 2}$

http://ie.lbl.gov/xray/xrf.htm

X-ray Fluorescence - Notation

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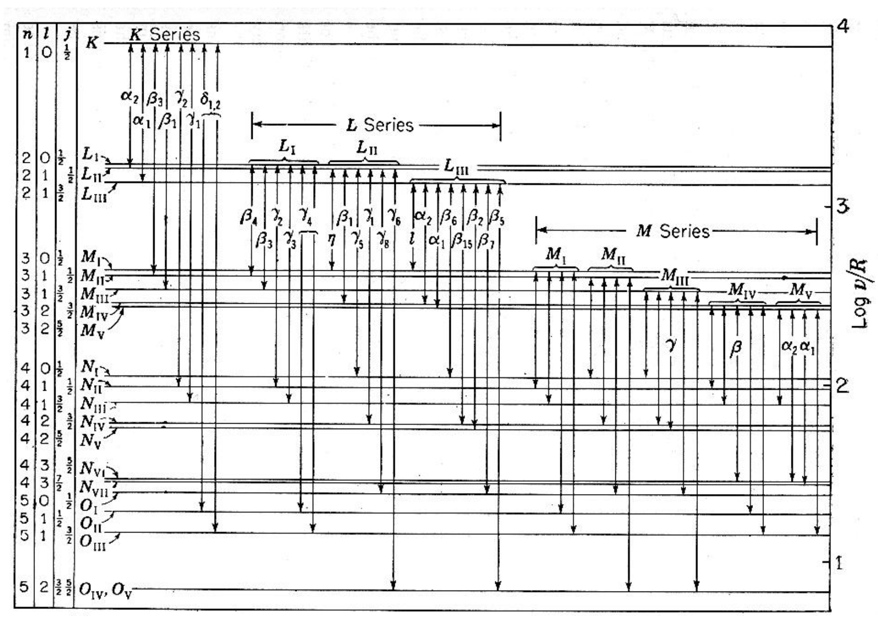


X-ray Fluorescence - Notation

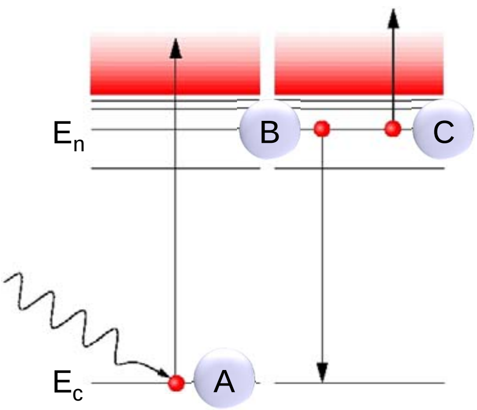
With Siegbahn notation: the scheme to assign the greek letters and numbers is not completely clear.

As a result of this less intuitive designation, a second notation from the International Union of Pure and Applied Chemistry (IUPAC) is recommended that clear identifies the transitions…

Zielniveau	Ursprungsniveau	IUPAC	Siegbahn
K	L_3	$K-L_3$	$K\alpha_1$
K	L_2	$K-L_2$	$L\alpha_2$
K	M_3	$K-M_3$	$K\beta_1$
K	M_2	$K-M_2$	$K\beta_3$
K	N_3	$K-N_3$	$K\beta_2'$
K	N_2	$K-N_2$	$K\beta_2''$
L_3	M_5	L_3-M_5	$L\alpha_1$
L_3	M_4	L_3-M_4	$L\alpha_2$
L_3	M_1	L_3-M_1	Ll
L_2	M_4	L_2-M_4	$L\beta_1$
L_2	M_1	L_2-M_1	$L\eta$
L_1	M_3	L_1-M_3	$L\beta_4$
L_1	M_2	L_1-M_2	$L\beta_5$
L_3	N_5	L_3-N_5	$L\beta_3$
L_3	N_4	L_3-N_4	$L\beta_{15}$
L_3	N_1	L_3-N_1	$L\beta_7$
L_2	N_4	L_2-N_4	$L\gamma_1$
L_2	N_1	L_2-N_1	$L\gamma_5$
L_1	N_3	L_1-N_3	$L\gamma_3$
L_1	N_2	L_1-N_2	$L\gamma_2$
M_5	N_7	M_5-N_7	$M\alpha_1$
M_5	N_6	M_5-N_6	$M\alpha_2$
M_4	N_6	M_4-N_6	$M\beta$
M_3	N_5	M_3-N_5	$M\gamma$

https://lp.uni-goettingen.de/get/text/6634

Auger Rules & Notation



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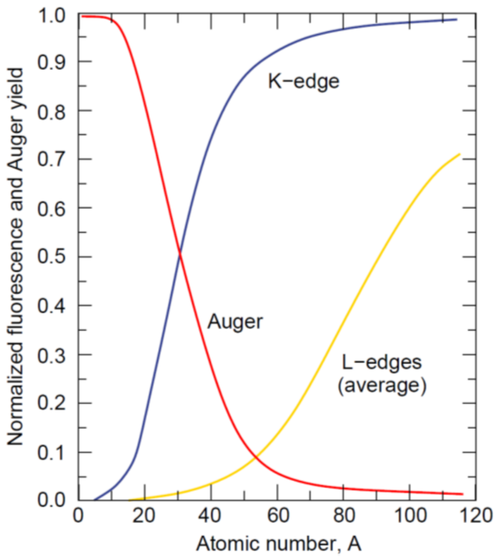
Fluorescence or Auger



Auger Yield and Fluorescence yields of the elements for K- and L- radiation

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