Today's outline - August 21, 2024

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Reading Assignment: Chapter 2.1–2.2

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Reading Assignment: Chapter 2.1–2.2

Homework Assignment #01:
Chapter 2: 2,3,5,6,8
due Wednesday, September 04, 2024

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- Scattering from a molecule
- Crystal lattice types
- The reciprocal lattice
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- X-ray absorption

Reading Assignment: Chapter 2.1–2.2

Homework Assignment #01:
Chapter 2: 2,3,5,6,8
due Wednesday, September 04, 2024

Homework Assignment #02:
Problems on Canvas
due Monday, September 16, 2024

Scattering from atoms: all effects

Scattering from an atom is built up from component quantities:

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Thomson scattering from a single electron $\quad -r_0 = -\dfrac{e^2}{4\pi\epsilon_0 mc^2}$

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atomic form factor $$f^0(\mathbf{Q}) = \int \rho(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r$$

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polarization factor $$P = \begin{cases} 1 \\ \sin^2\Psi \\ \frac{1}{2}(1+\sin^2\Psi) \end{cases}$$

$$-r_0 f(\mathbf{Q},\hbar\omega)\sin^2\Psi = -r_0\left[f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)\right]\sin^2\Psi$$

Computing atomic form factors

The atomic form factor is the Fourier transform of the electron distribution in the atom

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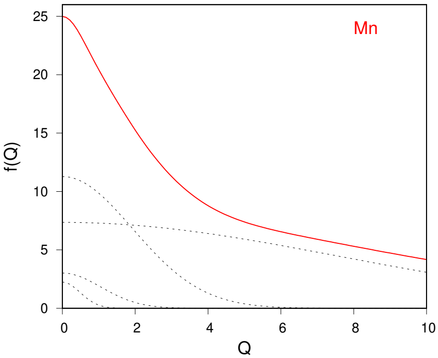

	a_1	b_1	a_2	b_2	a_3	b_3	a_4	b_4	c
Mn	11.2819	5.3409	7.3573	0.3432	3.0193	17.8674	2.2441	83.7543	1.0896

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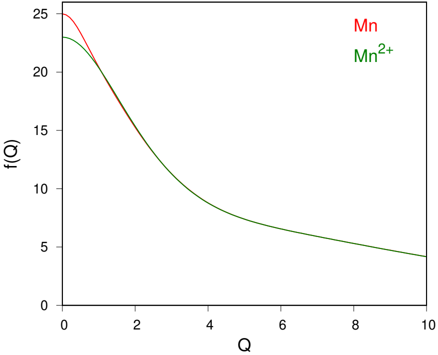

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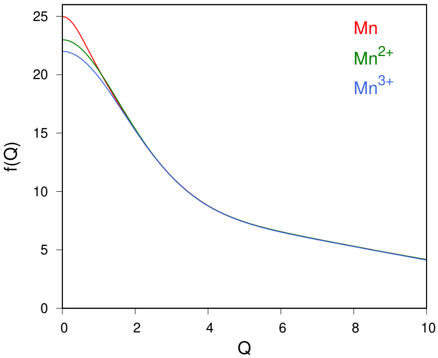

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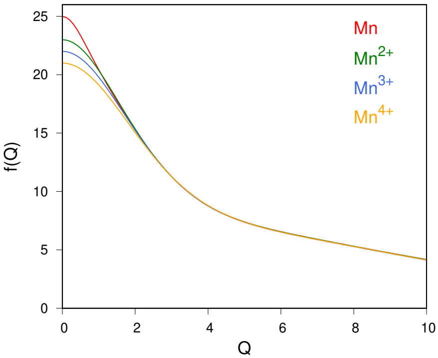

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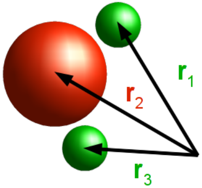

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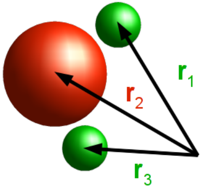

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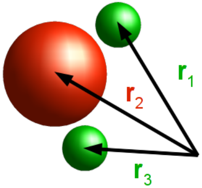

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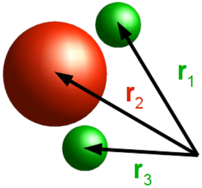

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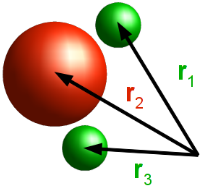

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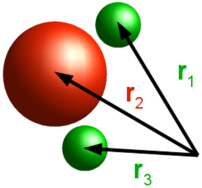

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Scattering from a crystal

and similarly, to a crystal lattice ...

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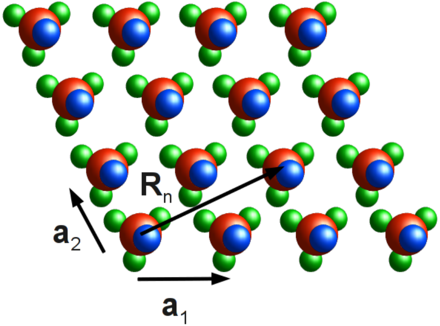

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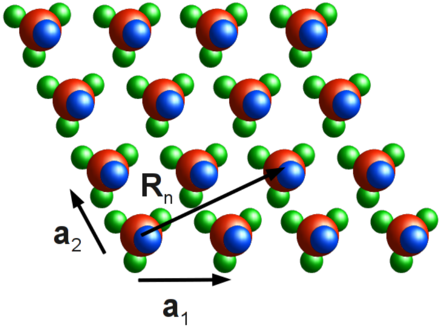

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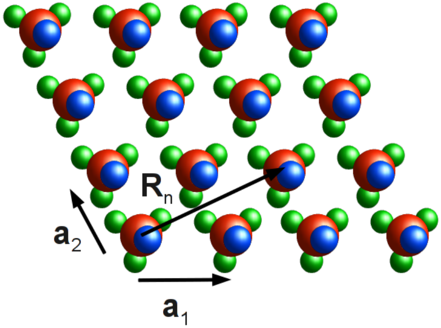

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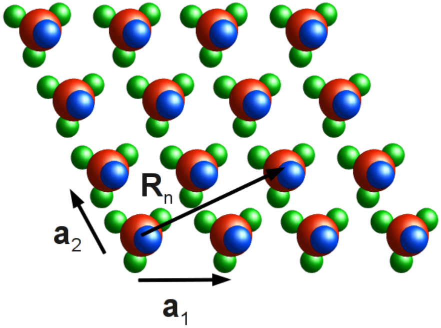

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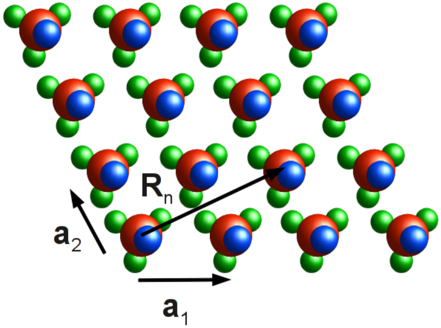

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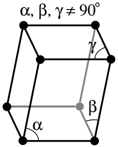
The lattice term, $\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}$, is a sum over a large number so it is always small unless $\mathbf{Q}\cdot\mathbf{R}_n = 2\pi m$ where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ is a real space lattice vector and m is an integer.

Crystal lattices

There are 7 possible real space lattices:



triclinic

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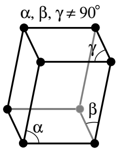

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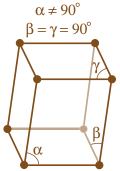

monoclinic

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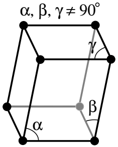

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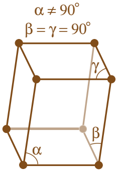

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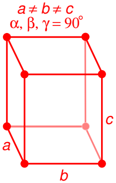

orthorhombic

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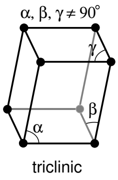

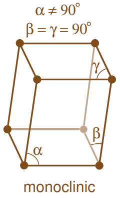

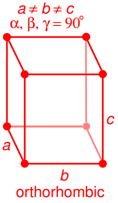

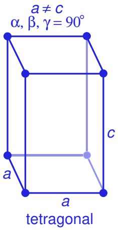

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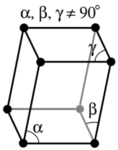
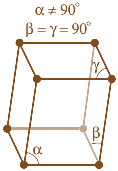


triclinic



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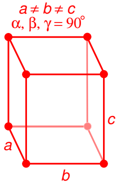
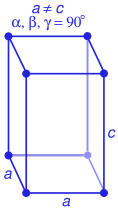
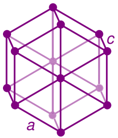


orthorhombic



tetragonal



hexagonal

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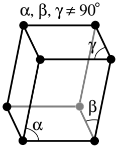
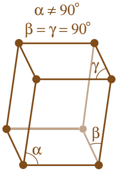
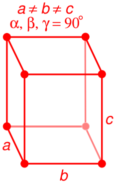


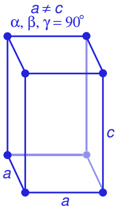
triclinic



monoclinic



orthorhombic



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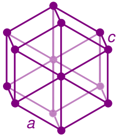

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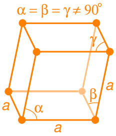

rhombohedral

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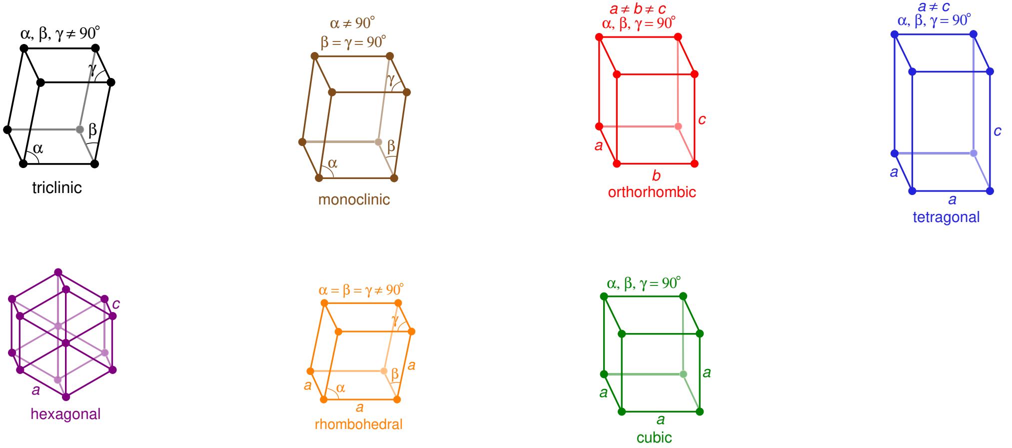
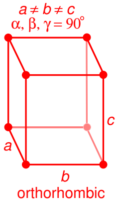


Lattice properties

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



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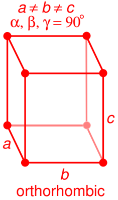

$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = b\hat{\mathbf{y}}, \quad \mathbf{a}_3 = c\hat{\mathbf{z}}$$

Lattice properties

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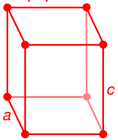

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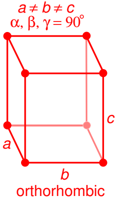

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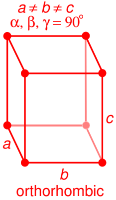

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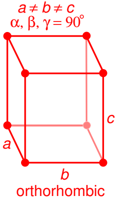

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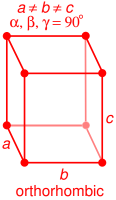

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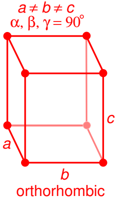

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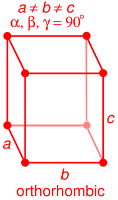

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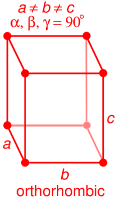

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As we shall see later, this Laue condition, is equivalent to the more typically used Bragg condition for diffraction: $2d \sin\theta = n\lambda$

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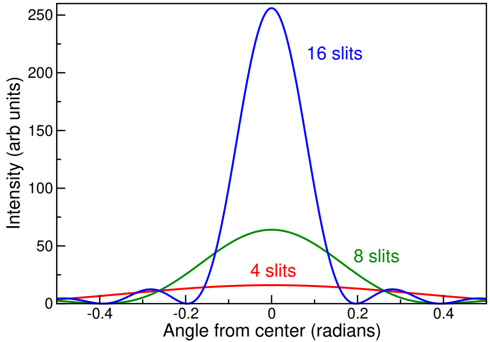

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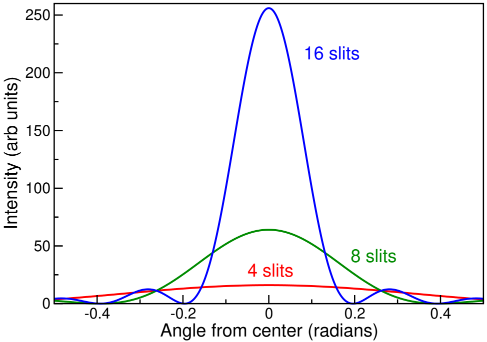

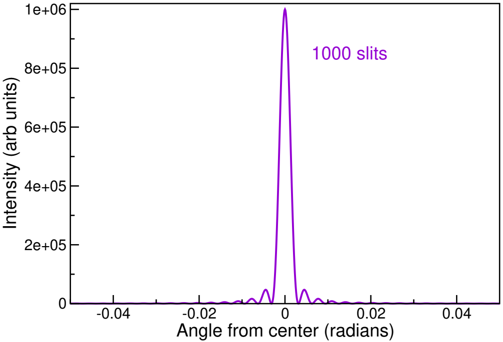

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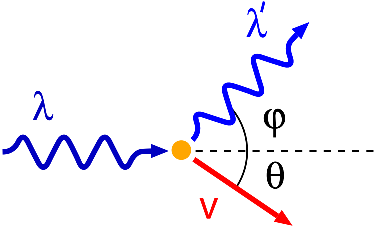

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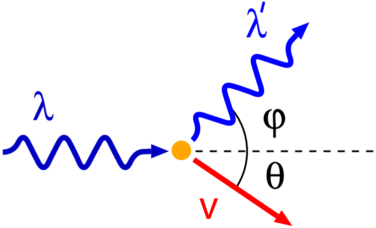

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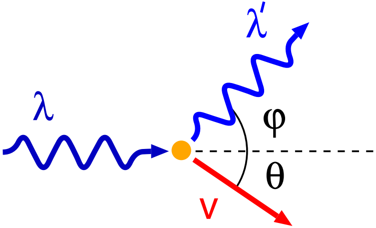

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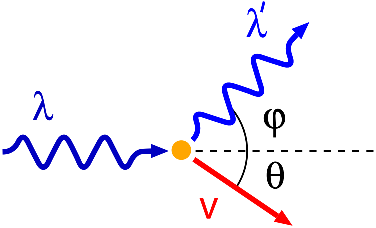

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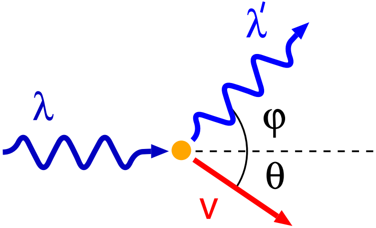

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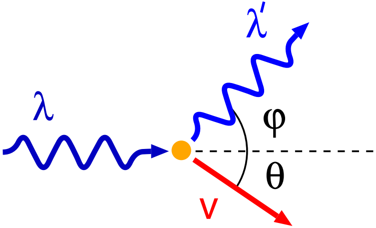

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$$mc^2 + \frac{hc}{\lambda} = \frac{hc}{\lambda'} + \gamma mc^2 \quad \text{(energy)}$$

Compton scattering

Consider a photon-electron collision

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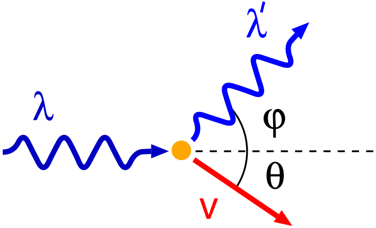

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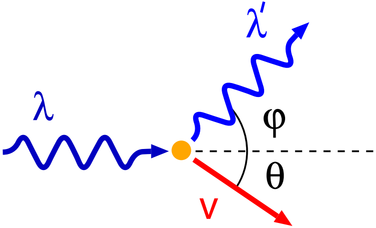

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Compton scattering derivation

squaring the momentum equations

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now add them together,

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Compton scattering derivation

squaring the momentum equations

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$$\frac{m^2 c^2 \beta^2}{1-\beta^2} = \frac{m^2 v^2}{1-\beta^2} = \frac{h^2}{\lambda^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi + \frac{h^2}{\lambda'^2}$$

Compton scattering derivation (cont.)

Now take the energy equation and square it,

$$\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2 = \gamma^2 m^2 c^4 = \frac{m^2 c^4}{1-\beta^2}$$

Compton scattering derivation (cont.)

Now take the energy equation and square it, then solve it for β^2

$$\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2 = \gamma^2 m^2 c^4 = \frac{m^2 c^4}{1-\beta^2}$$

$$\beta^2 = 1 - \frac{m^2 c^4}{\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2}$$

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Now take the energy equation and square it, then solve it for β^2 which is substituted into the equation from the momentum.

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Compton scattering derivation (cont.)

After expansion,

$$\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi = \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2$$

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Compton scattering derivation (cont.)

After expansion, cancellation,

$$\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi = \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2$$

$$= \cancel{m^2c^2} + \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2mch}{\lambda} - \frac{2mch}{\lambda'} + \frac{2h^2}{\lambda\lambda'} - \cancel{m^2c^2}$$

$$= 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) + \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}$$

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Compton scattering derivation (cont.)

After expansion, cancellation, and rearrangement, we obtain

$$\cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\cos\phi = \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2$$

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$$\cancel{\frac{h^2}{\lambda^2}} + \cancel{\frac{h^2}{\lambda'^2}} - \frac{2h^2}{\lambda\lambda'}\cos\phi = \left(mc + \frac{h}{\lambda} - \frac{h}{\lambda'}\right)^2 - m^2c^2$$

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$$\Delta\lambda = \frac{h}{mc}(1-\cos\phi)$$

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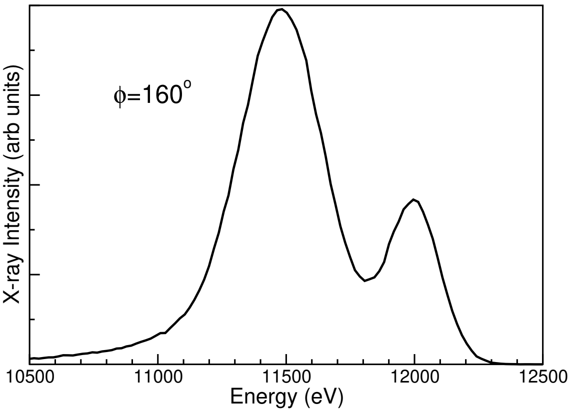
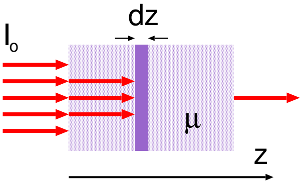


Scattering of 12 keV x-rays from a silicon wafer at 160° with a bent crystal wavelength dispersive analyzer

X-ray absorption



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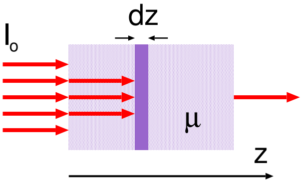

For absorption coefficient μ and thickness dz the x-ray intensity is attenuated as

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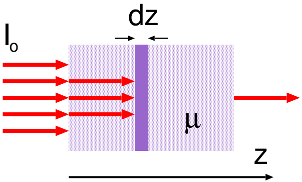

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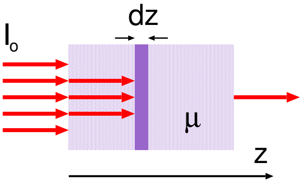

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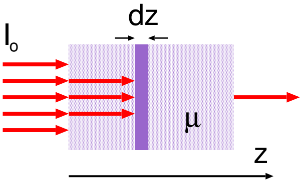

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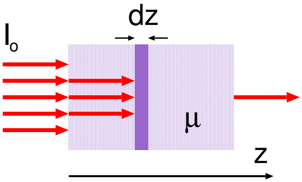

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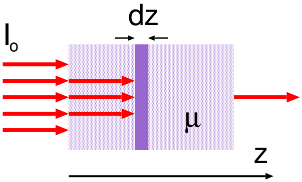

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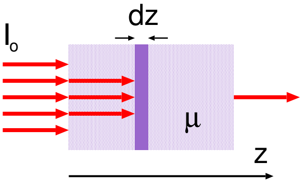

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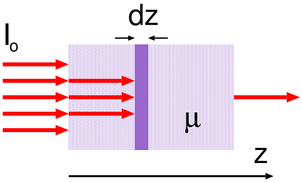

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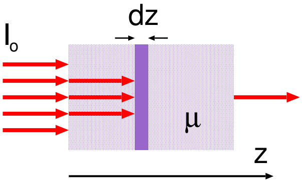

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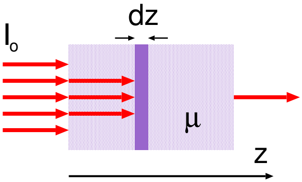

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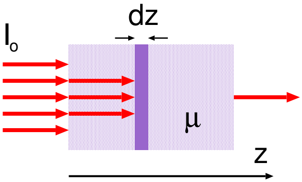

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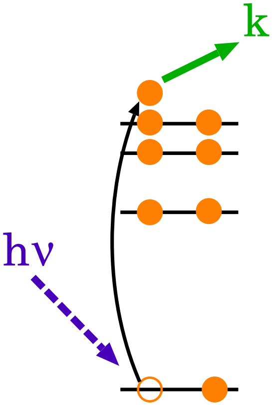
This is just Beer's law with an absorption coefficient which depends on x-ray parameters.

Absorption event



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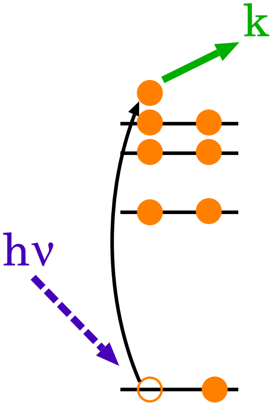
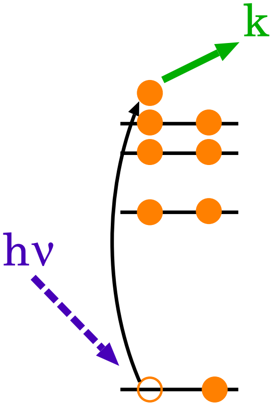


X-ray is absorbed by an atom

Absorption event



X-ray is absorbed by an atom

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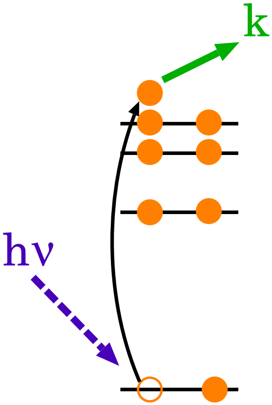
Absorption event

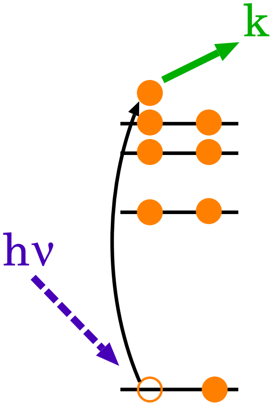


X-ray is absorbed by an atom

Energy is transferred to a core electron

Electron escapes atomic potential into the continuum

Absorption event



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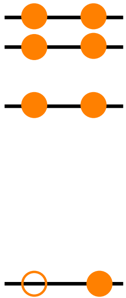
Electron escapes atomic potential into the continuum

Ion remains with a core-hole

Fluorescence emission

An ion with a core-hole is quite unstable ($\approx 10^{-15}$s)



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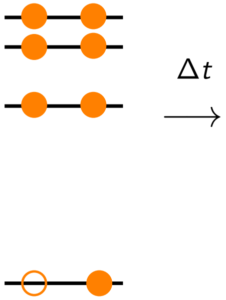

After a short time a higher level electron will drop down in energy to fill the core hole

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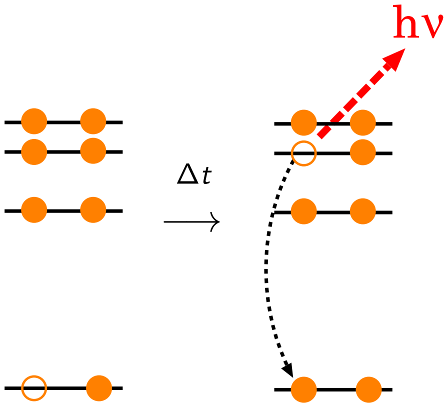

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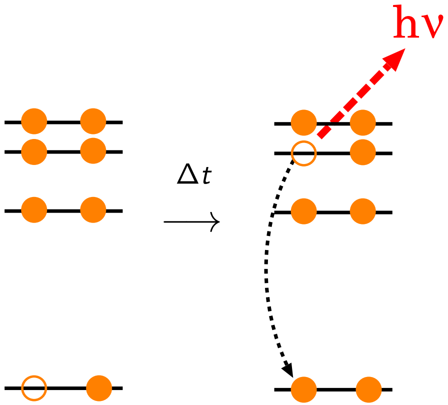

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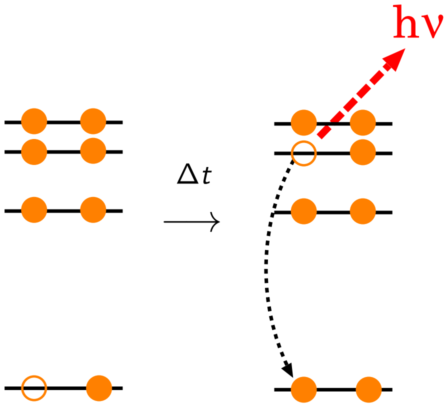

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Energy is liberated in the form of a fluorescence photon

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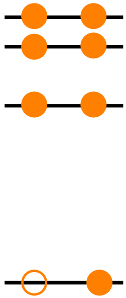
The result is a cascade of fluorescence photons which are characteristic of the absorbing atom

Auger emission

While fluorescence is the most probable method of core-hole relaxation there are other possible mechanisms



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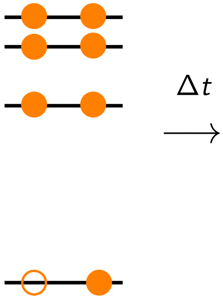

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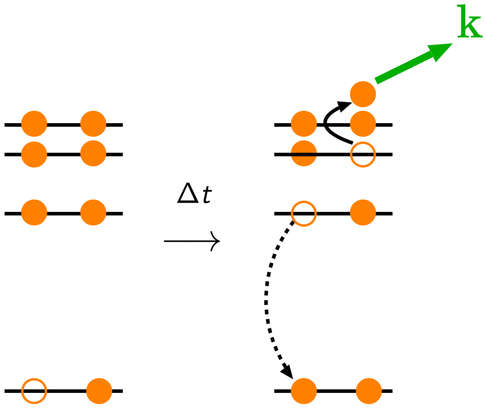

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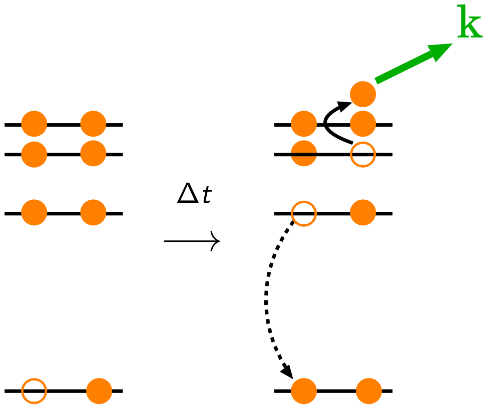

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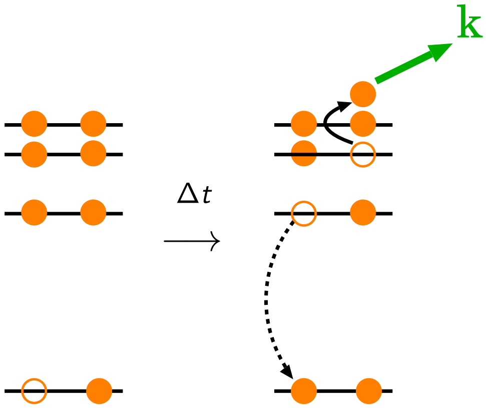

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The energy liberated causes the secondary emission of an electron

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So that the secondary electron is accompanied by fluorescence emissions at lower energies

Absorption coefficient

The absorption coefficient μ,

$$\mu \sim \frac{\quad}{\quad}$$

Absorption coefficient

The absorption coefficient μ, depends strongly on the x-ray energy E,

$$\mu \sim \frac{}{E^3}$$

Absorption coefficient

The absorption coefficient μ, depends strongly on the x-ray energy E, the atomic number of the absorbing atoms Z,

$$\mu \sim \frac{Z^4}{E^3}$$

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The absorption coefficient μ, depends strongly on the x-ray energy E, the atomic number of the absorbing atoms Z, as well as the density ρ,

$$\mu \sim \frac{\rho Z^4}{E^3}$$

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The absorption coefficient μ, depends strongly on the x-ray energy E, the atomic number of the absorbing atoms Z, as well as the density ρ, and atomic mass A:

$$\mu \sim \frac{\rho Z^4}{A E^3}$$

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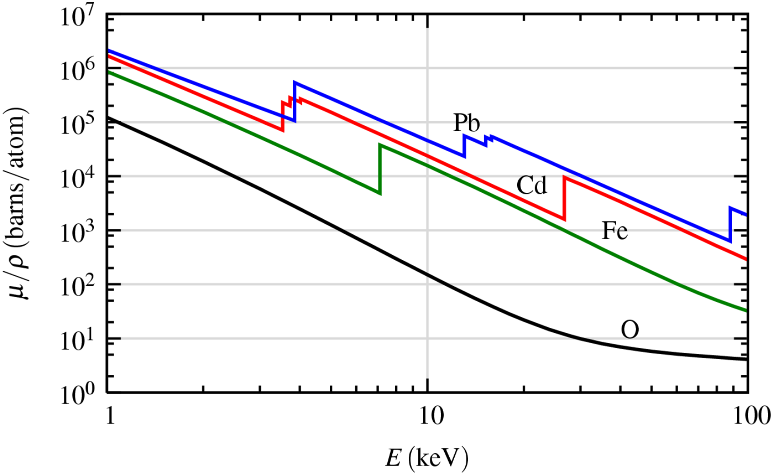
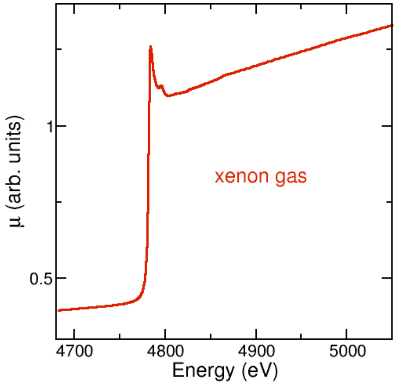


Absorption coefficient

Isolated gas atoms show a sharp jump and a smooth curve



Absorption coefficient

Isolated gas atoms show a sharp jump and a smooth curve but atoms in a solid or liquid show fine structure after the absorption edge called XANES and EXAFS