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Scattering from a crystal (review)

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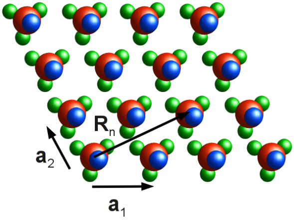

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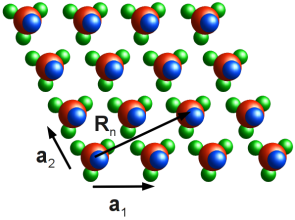

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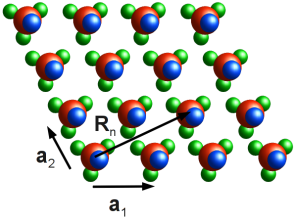

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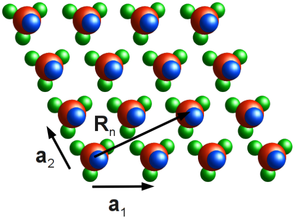

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The lattice term, $\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}$, is a sum over a large number so it is always small unless $\mathbf{Q}\cdot\mathbf{R}_n = 2\pi m$ where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ is a real space lattice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

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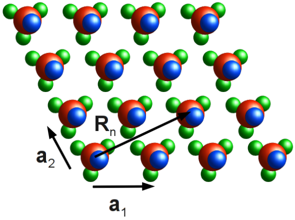

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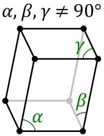
This condition is fulfilled only when $\mathbf{Q}$ is a reciprocal lattice vector.

Crystal lattices

There are 7 possible real space lattices: triclinic,



Crystal lattices

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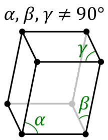

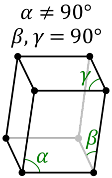

Crystal lattices

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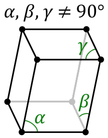
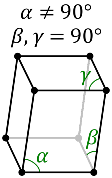
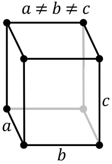
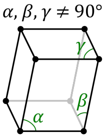


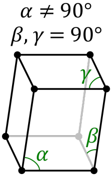


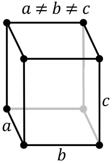


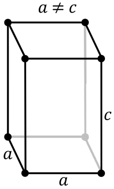
Crystal lattices

There are 7 possible real space lattices: triclinic, monoclinic, orthorhombic, tetragonal,









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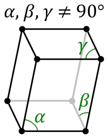

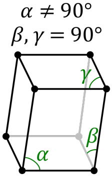

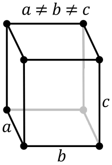

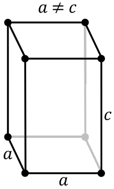

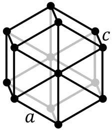

Crystal lattices

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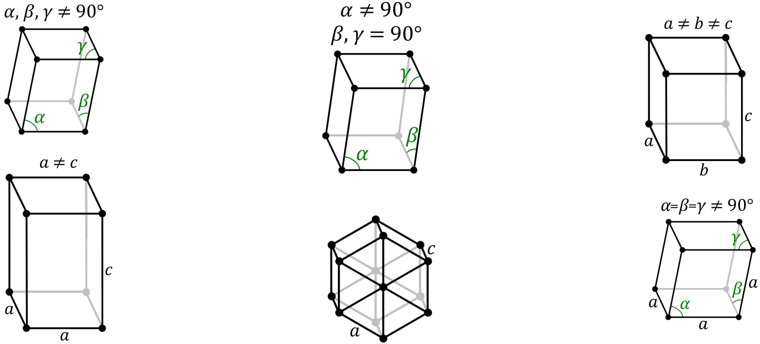

Crystal lattices

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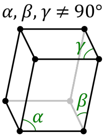
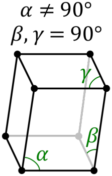
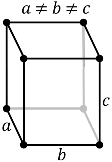
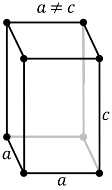
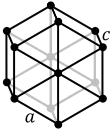
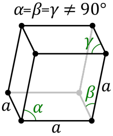


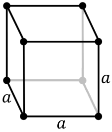






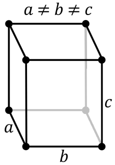






Lattice properties

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



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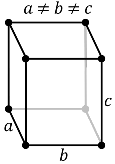

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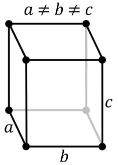

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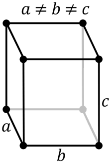

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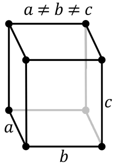

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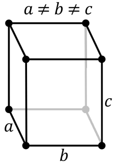

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A simple way of calculating the volume of the unit cell!

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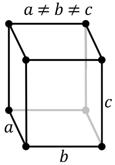

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This unit cell is repeated infintely in 3-dimensions and thus, the location of each lattice point can be calculated relative to any arbitrary lattice point designated as the origin.

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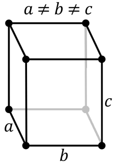

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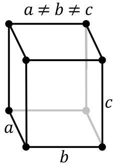

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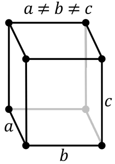

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Each lattice point is at the end of a lattice vector, $\mathbf{R}_n$ and a crystal is made by putting a molecule at each lattice point.

$$\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

Reciprocal lattice

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In analogy to $\mathbf{R}_n$, we can construct an arbitrary reciprocal space lattice vector $\mathbf{G}_{hkl}$

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$$\mathbf{a}_3^* = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)} = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{V}$$

In analogy to $\mathbf{R}_n$, we can construct an arbitrary reciprocal space lattice vector $\mathbf{G}_{hkl}$

$$\mathbf{G}_{hkl} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$$

Reciprocal lattice

For any lattice in real space, it is useful to construct what is called a reciprocal space lattice.

Define the reciprocal lattice vectors in terms of the real space unit vectors

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V}$$
$$\mathbf{a}_2^* = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)} = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V}$$
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$$\mathbf{G}_{hkl} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$$

where h, k, and l are integers called Miller indices

Laue condition

Because of the construction of the reciprocal lattice

Laue condition

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$\mathbf{G}_{hkl} \cdot \mathbf{R}_n$

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$$\mathbf{G}_{hkl} \cdot \mathbf{R}_n = (n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3) \cdot (h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*)$$

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and therefore, the crystal scattering factor

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$$\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}$$

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so a significant number of molecules scatter *in phase* with each other

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

Multiple slit interference

A crystal is, therefore, a diffraction grating with $\sim 10^{20}$ slits!

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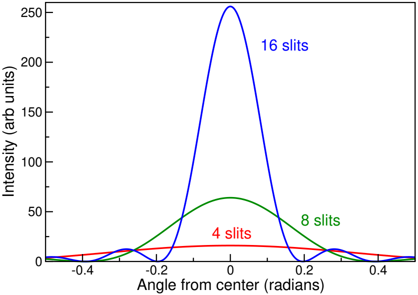

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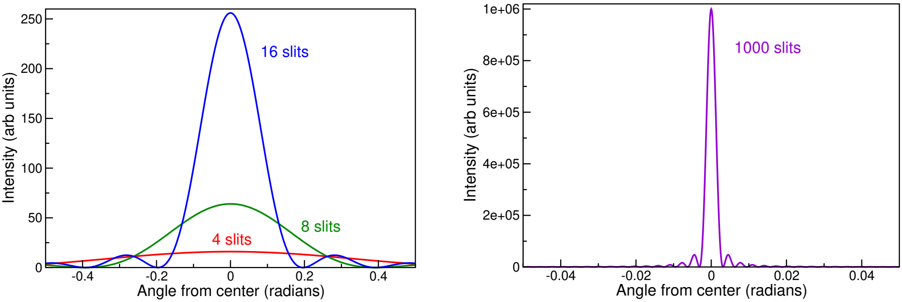

Compton scattering

A photon-electron collision

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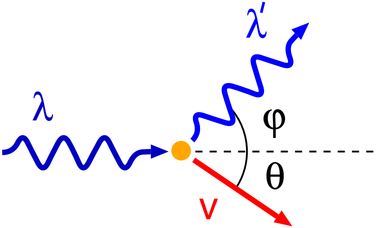

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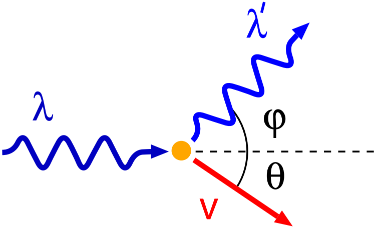

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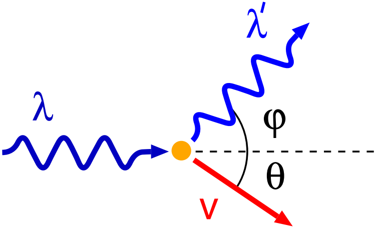

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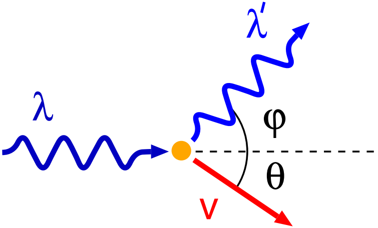

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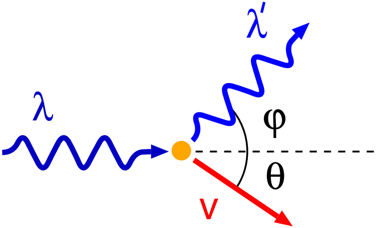

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Treat the electron relativistically and conserve energy and momentum

Compton scattering

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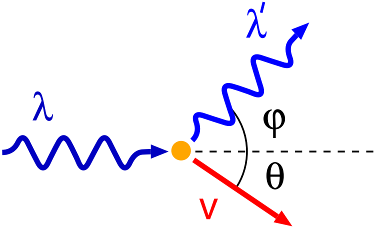

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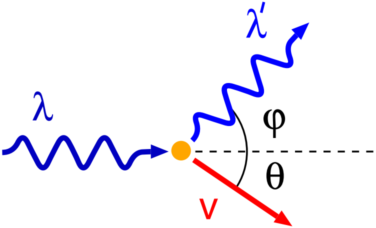
Treat the electron relativistically and conserve energy and momentum

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

A photon-electron collision



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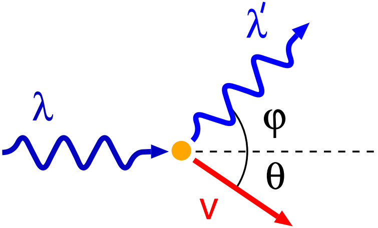
Treat the electron relativistically and conserve energy and momentum

$$mc^2 + \frac{hc}{\lambda} = \frac{hc}{\lambda'} + \gamma mc^2 \quad \text{(energy)}$$
$$\frac{h}{\lambda} = \frac{h}{\lambda'}\cos\phi + \gamma mv\cos\theta \quad \text{(x-axis)}$$

Compton scattering

A photon-electron collision



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$$0 = \frac{h}{\lambda'}\sin\phi + \gamma mv\sin\theta \quad \text{(y-axis)}$$

Compton scattering derivation

squaring the momentum equations

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$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \cos^2\theta$$

Compton scattering derivation

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$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \cos^2\theta$$

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Compton scattering derivation

squaring the momentum equations

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now add them together,

$$\gamma^2 m^2 v^2 \left(\sin^2\theta + \cos^2\theta\right) = \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 + \left(-\frac{h}{\lambda'}\sin\phi\right)^2$$

Compton scattering derivation

squaring the momentum equations

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now add them together, substitute $\sin^2\theta + \cos^2\theta = 1$, expand the squares,

$$\gamma^2 m^2 v^2 \left(\sin^2\theta + \cos^2\theta\right) = \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 + \left(-\frac{h}{\lambda'}\sin\phi\right)^2$$

$$\gamma^2 m^2 v^2 = \frac{h^2}{\lambda^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi + \frac{h^2}{\lambda'^2}\sin^2\phi + \frac{h^2}{\lambda'^2}\cos^2\phi$$

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squaring the momentum equations

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now add them together, substitute $\sin^2\theta + \cos^2\theta = 1$, expand the squares, and $\sin^2\phi + \cos^2\phi = 1$, then rearrange

$$\gamma^2 m^2 v^2 \left(\sin^2\theta + \cos^2\theta\right) = \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 + \left(-\frac{h}{\lambda'}\sin\phi\right)^2$$

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

Compton scattering derivation

squaring the momentum equations

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now add them together, substitute $\sin^2\theta + \cos^2\theta = 1$, expand the squares, and $\sin^2\phi + \cos^2\phi = 1$, then rearrange and substitute $v = \beta c$

$$\gamma^2 m^2 v^2 \left(\sin^2\theta + \cos^2\theta\right) = \left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 + \left(-\frac{h}{\lambda'}\sin\phi\right)^2$$

$$\gamma^2 m^2 v^2 = \frac{h^2}{\lambda^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi + \frac{h^2}{\lambda'^2}\sin^2\phi + \frac{h^2}{\lambda'^2}\cos^2\phi$$

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

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

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

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

Compton scattering derivation (cont.)

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

Compton scattering derivation (cont.)

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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$$\begin{aligned}\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi &= \frac{m^2 c^2 \beta^2}{1-\beta^2} \\ &= \frac{1}{c^2}\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2 - m^2 c^2\end{aligned}$$

Compton scattering derivation (cont.)

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

Compton scattering derivation (cont.)

After expansion,

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

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

Compton scattering derivation (cont.)

After expansion, cancellation,

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

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

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

Compton scattering derivation (cont.)

After expansion, cancellation,

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

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

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Compton scattering derivation (cont.)

After expansion, cancellation, and rearrangement, we obtain

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

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

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

$$\frac{2h^2}{\lambda\lambda'}(1 - \cos\phi) = 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)$$

Compton scattering derivation (cont.)

After expansion, cancellation,

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

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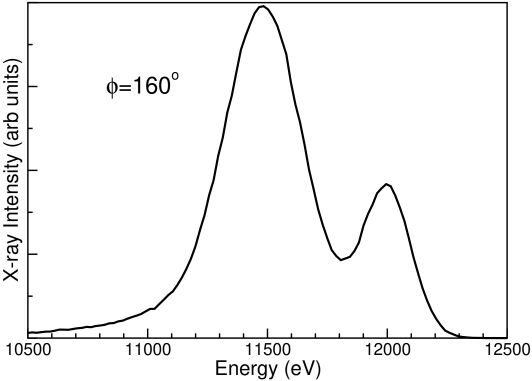

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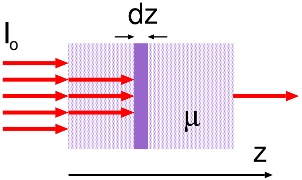

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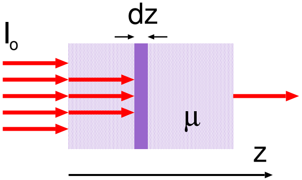

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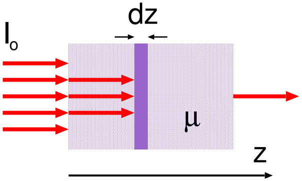

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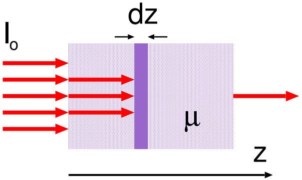

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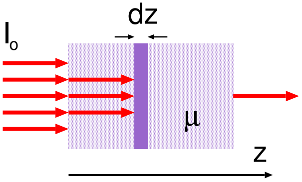

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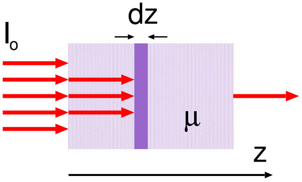

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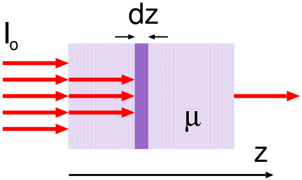

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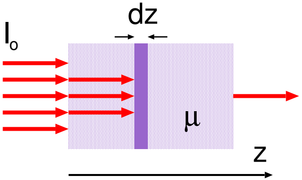

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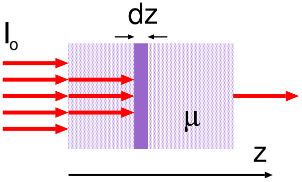

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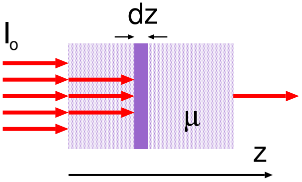

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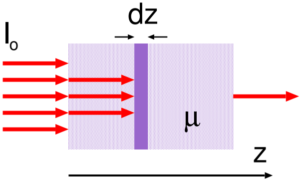

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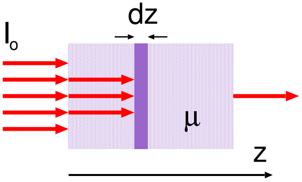

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This is just Beer's law with an absorption coefficient which depends on x-ray parameters.

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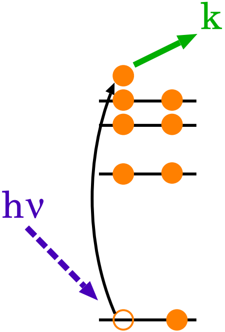

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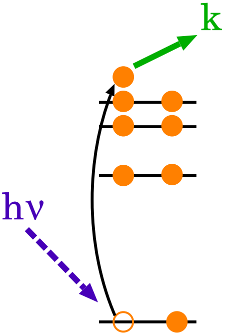

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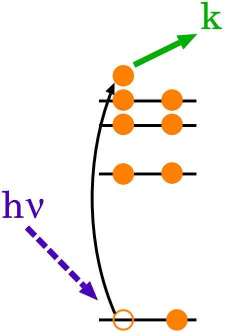

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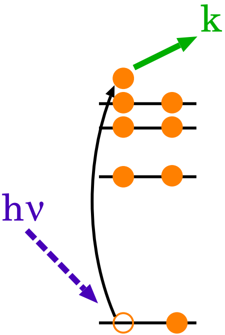

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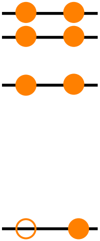
- Ion remains with a core-hole

Fluorescence emission

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



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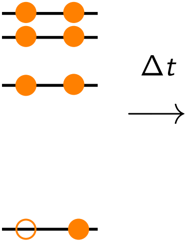

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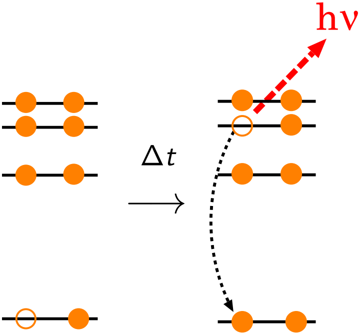

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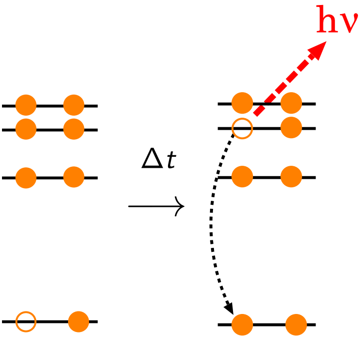

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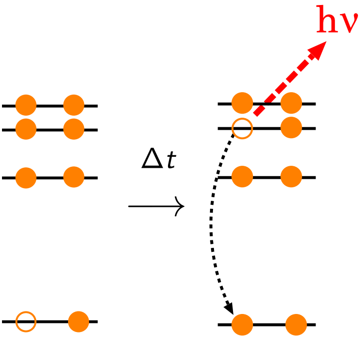

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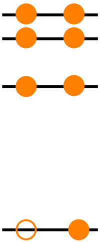
- The result is a cascade of fluorescence photons which are characteristic of the absorbing atom

Auger emission

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



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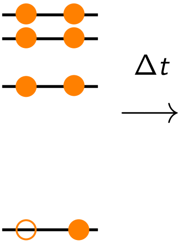

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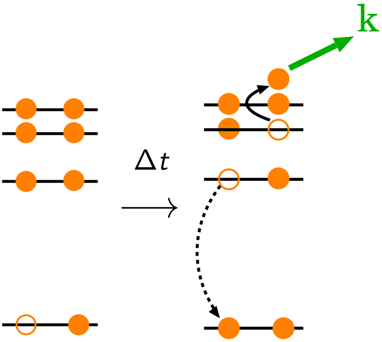

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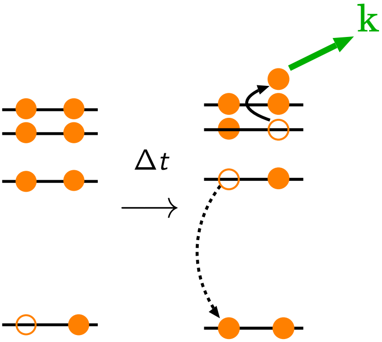

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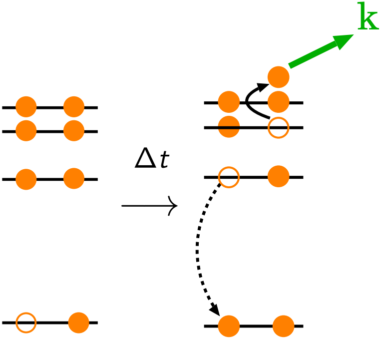

- In the Auger process, a higher level electron will drop down in energy to fill the core hole
- The energy liberated causes the secondary emission of an electron
- This leaves two holes which then filled from higher shells
- So that the secondary electron is accompanied by fluorescence emissions at lower energies

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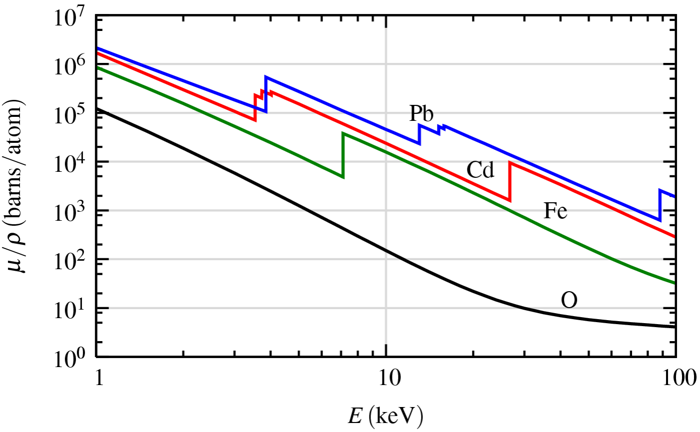

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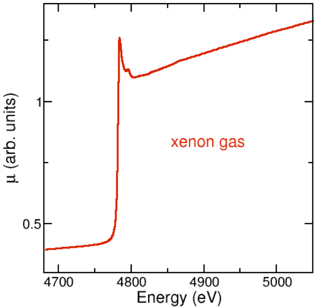

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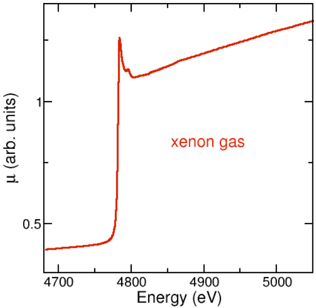

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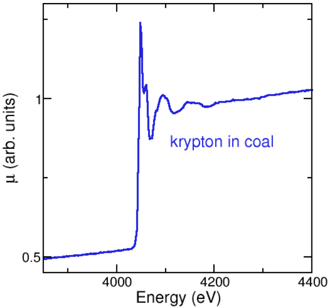

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If the compound is made up of x_j atoms with atomic mass M_j and has a molecular mass M_c and density ρ_c, we can write:

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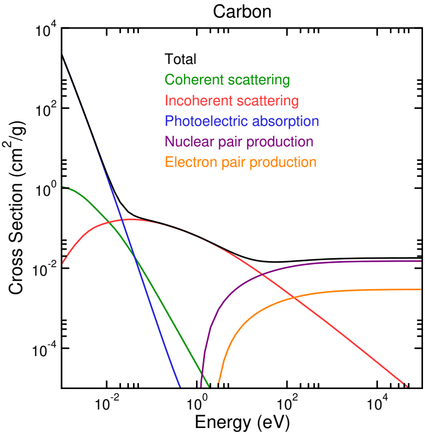

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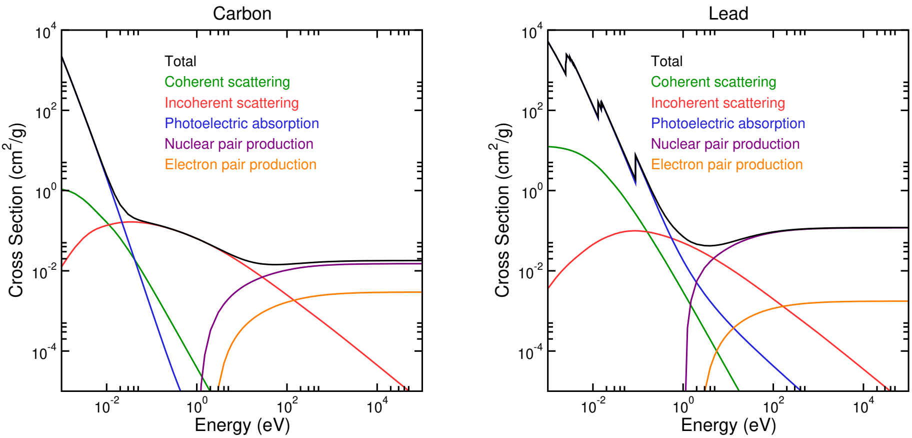

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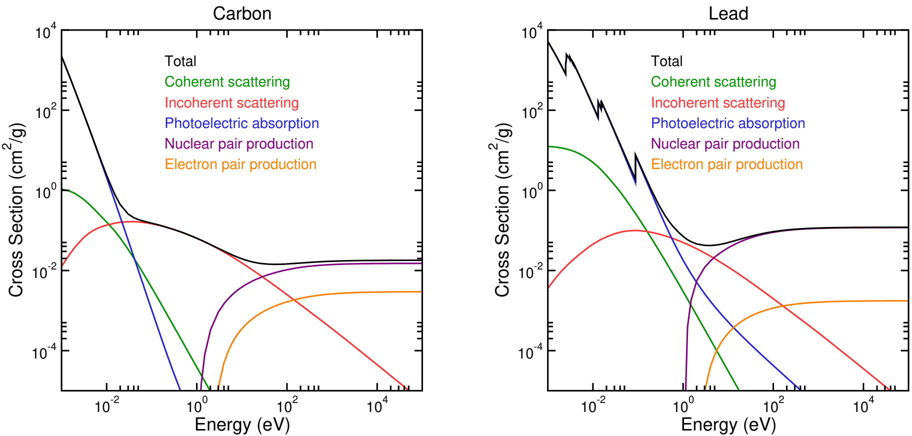

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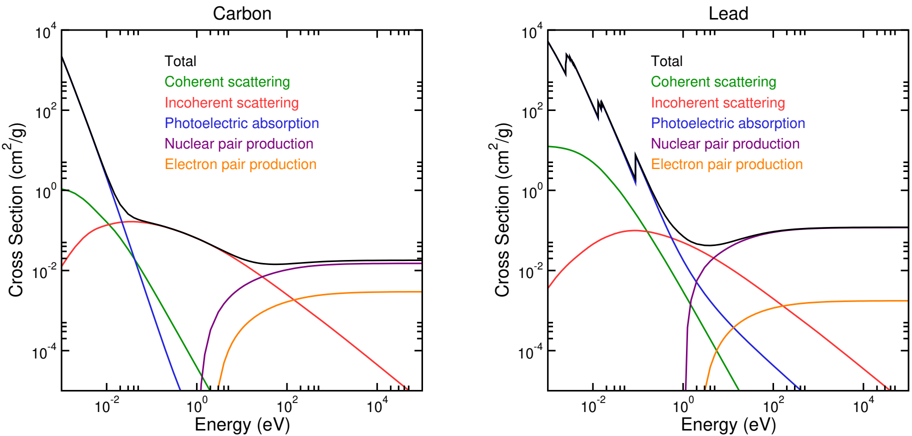

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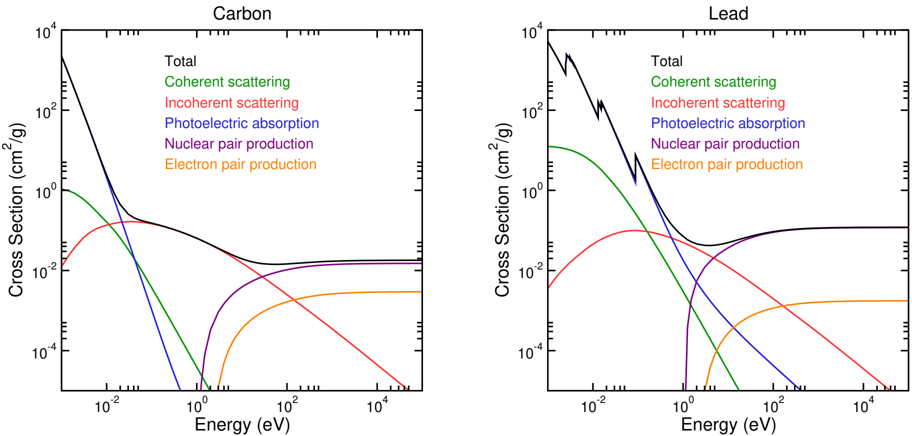

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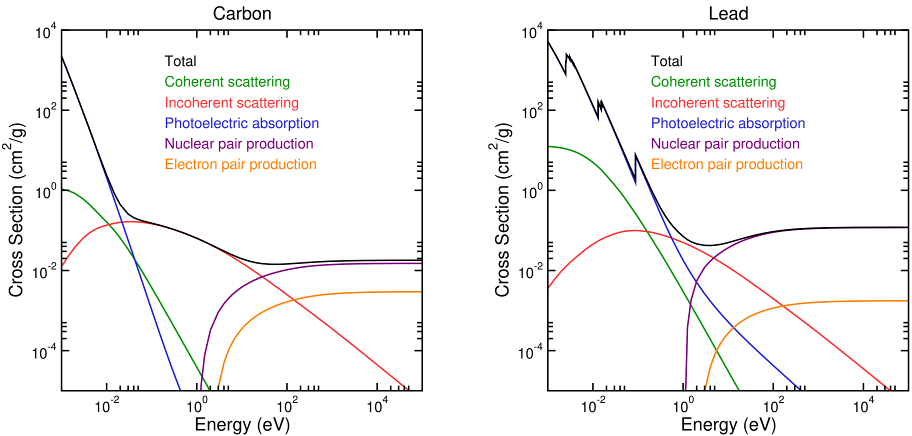

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