Today's Outline - January 15, 2015

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- Coherence of x-ray sources

Scattering from atoms: all effects

Scattering from an atom is built up from component quantities:

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

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anomalous scattering terms $f'(\hbar\omega) + if''(\hbar\omega)$

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

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

Scattering from molecules

extending to a molecule ...

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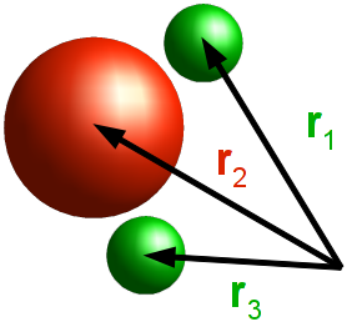

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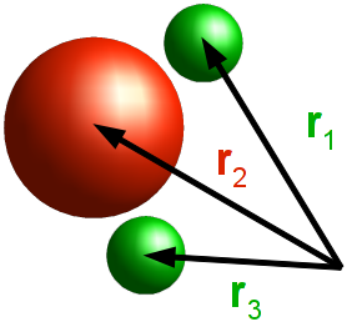

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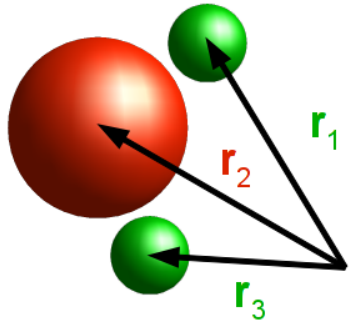

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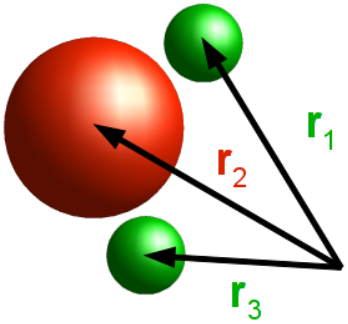

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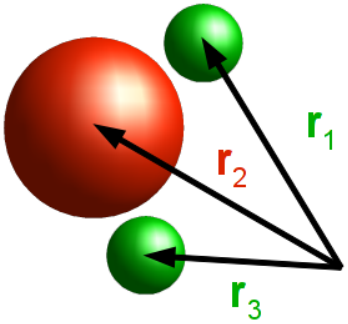

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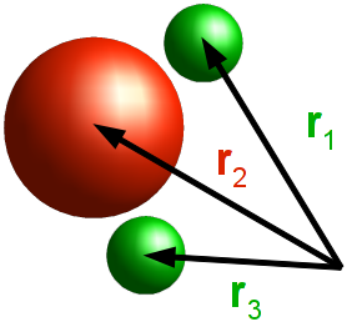

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Scattering from a crystal

and similarly, to a crystal lattice ...

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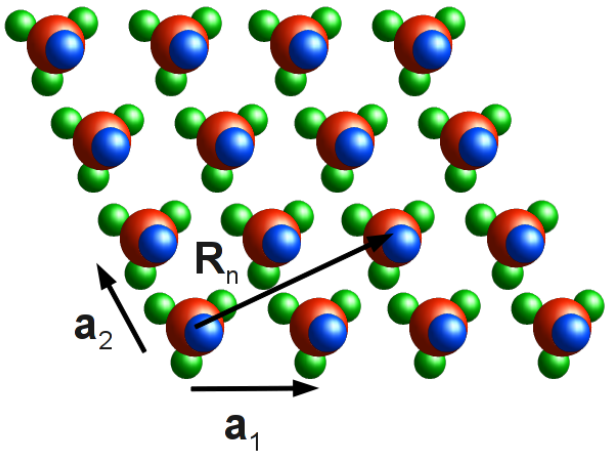

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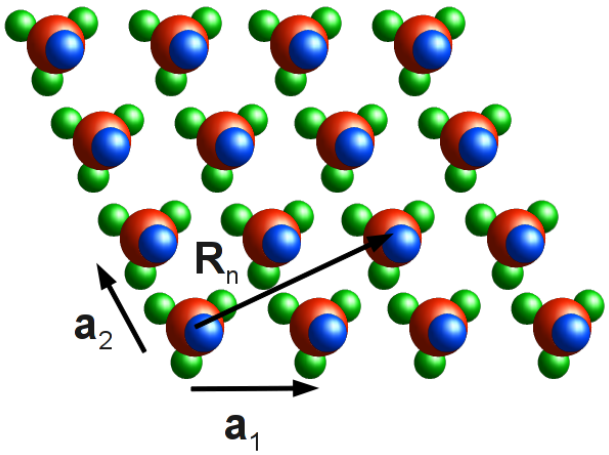

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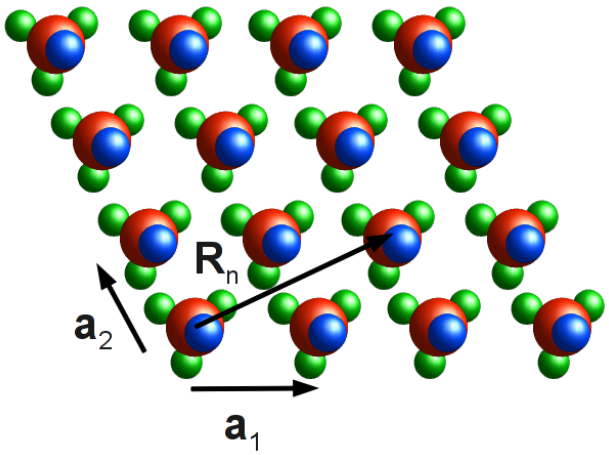

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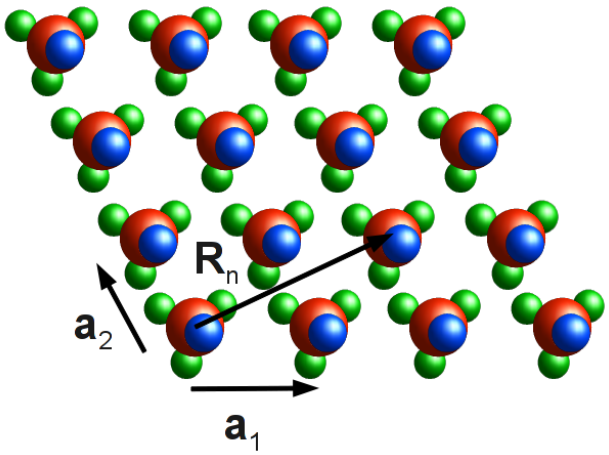

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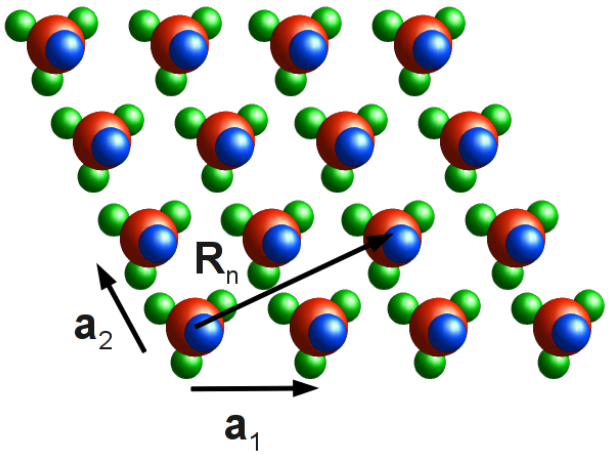

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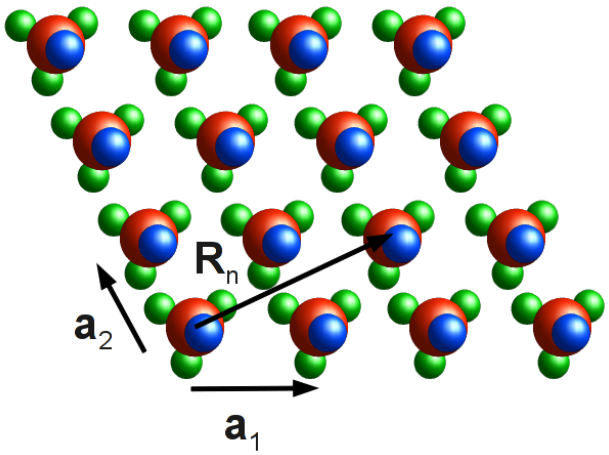

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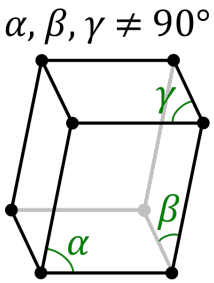
Crystal lattices

There are 7 possible real space lattices: triclinic,



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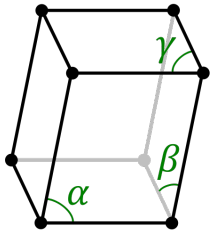
There are 7 possible real space lattices: triclinic, monoclinic,

$\alpha, \beta, \gamma \neq 90°$



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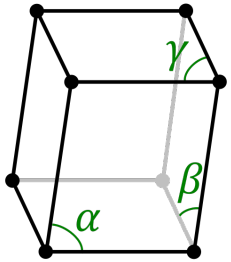
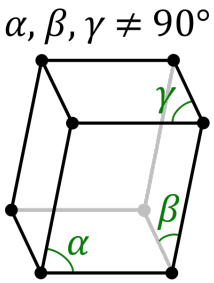
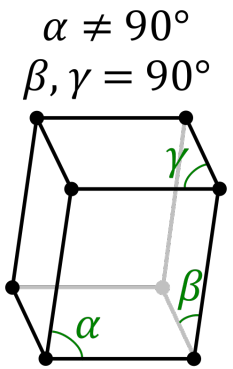
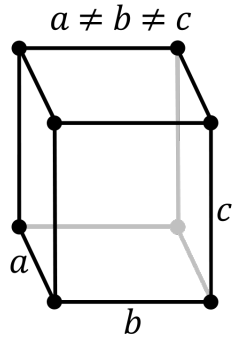


Crystal lattices

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







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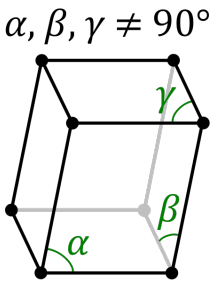
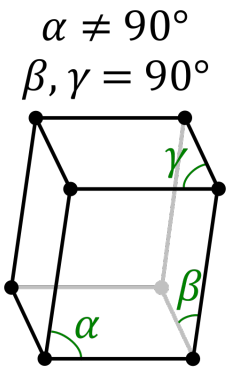
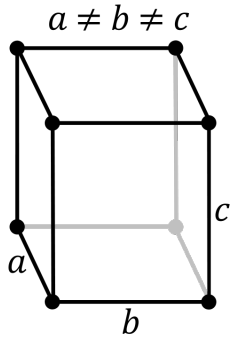
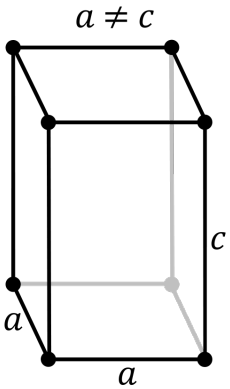


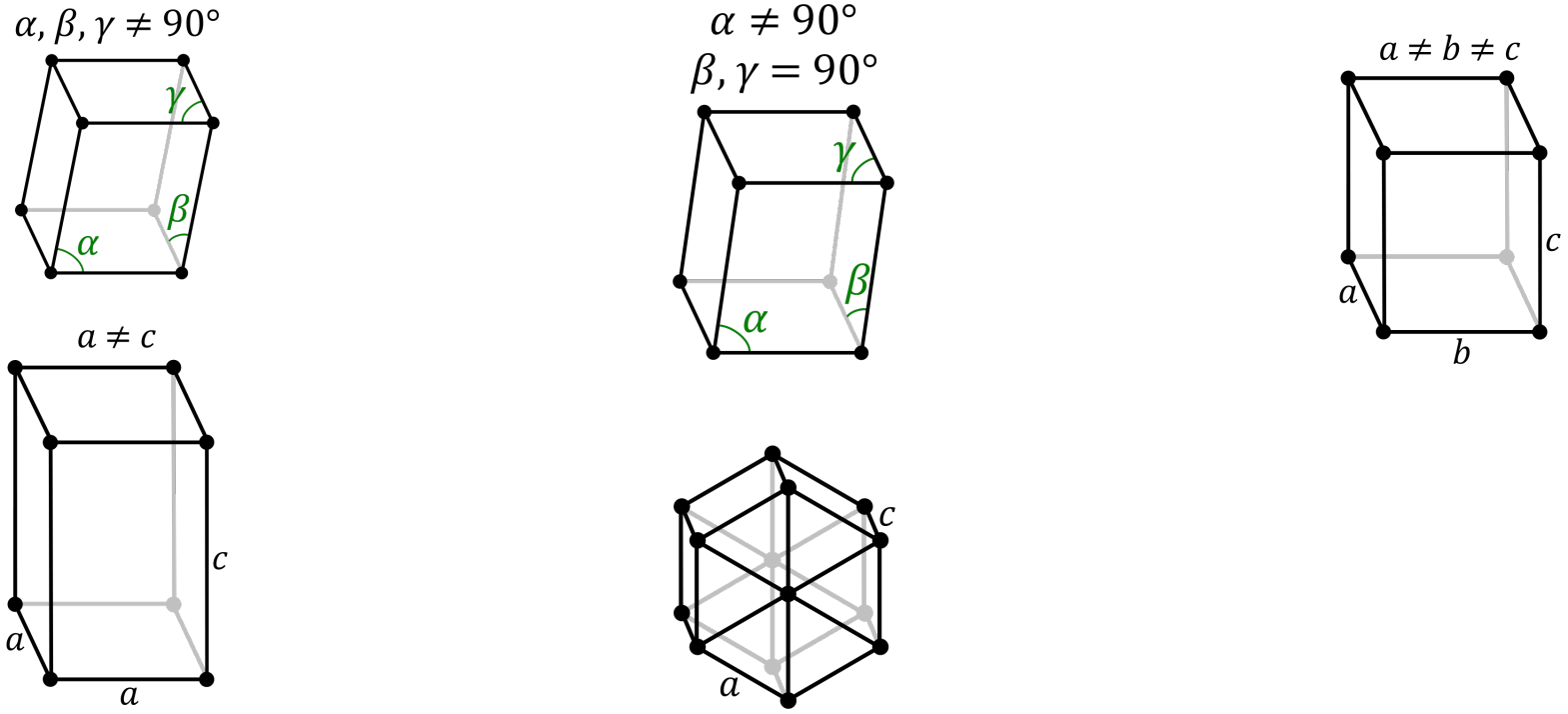






Crystal lattices

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



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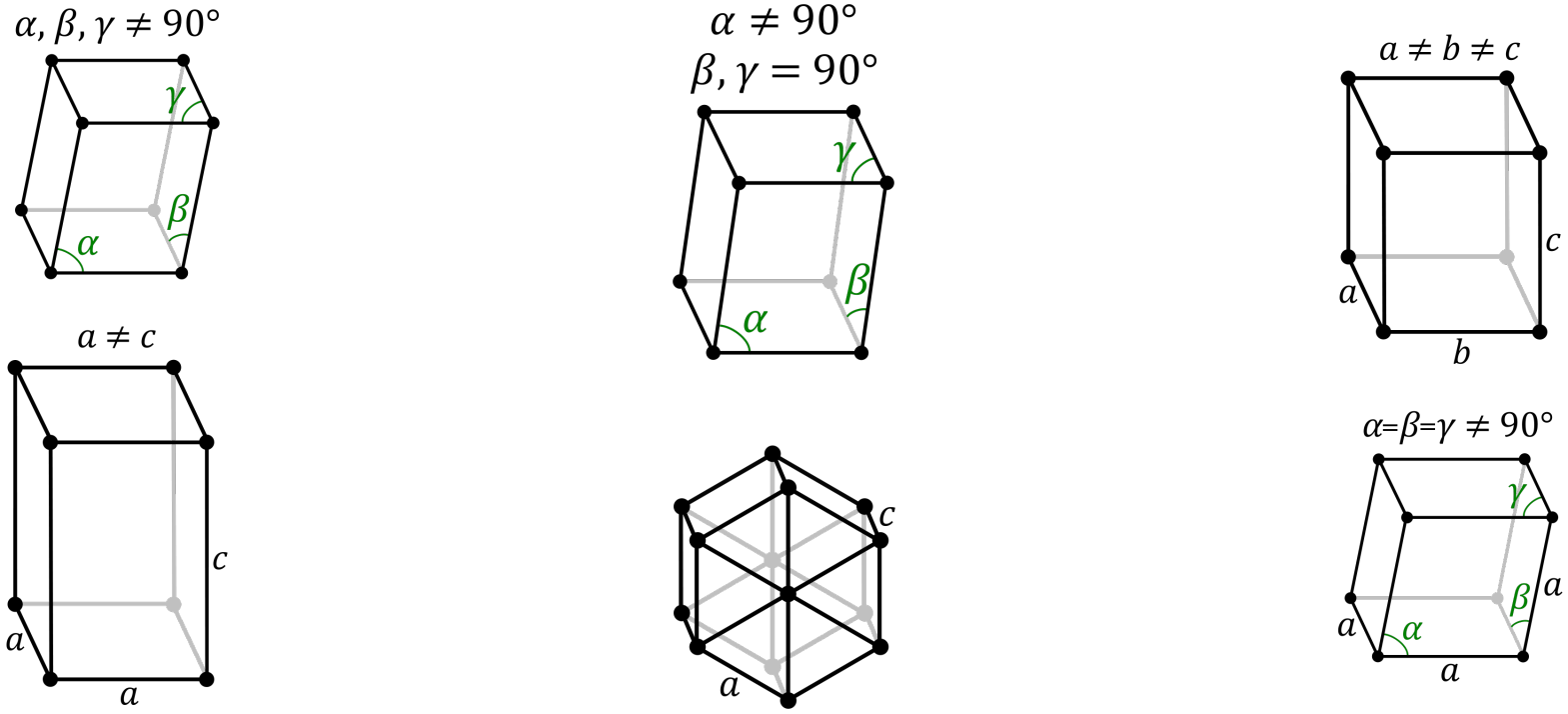

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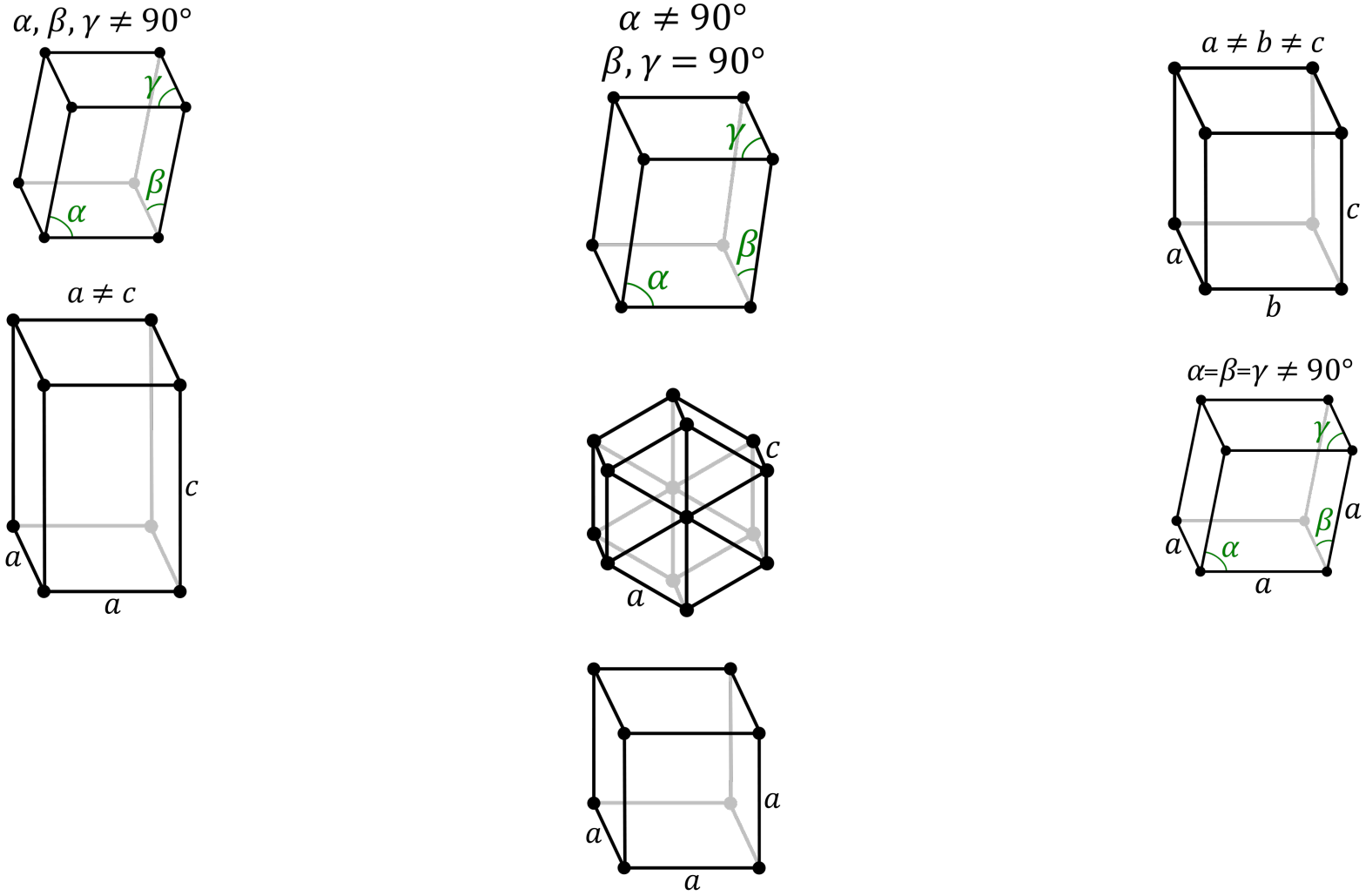
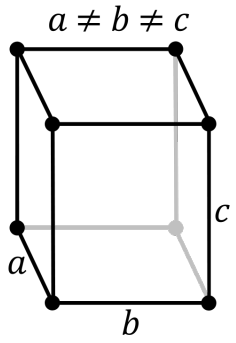


Lattice volume

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



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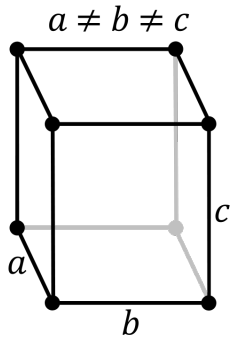

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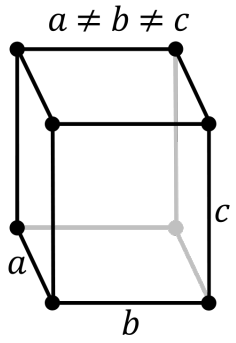

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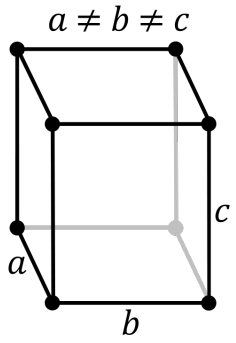

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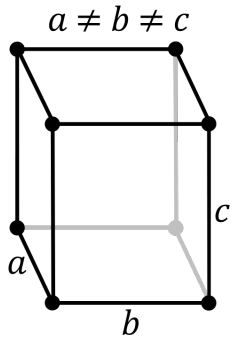

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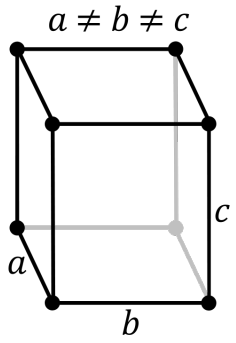

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A simple way of calculating the volume of the unit cell!

Reciprocal lattice

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

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

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

Reciprocal lattice

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

$$\mathbf{a}_1^* = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V}$$
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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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where h, k, and l are integers called Miller indices

Laue condition

Because of the construction of the reciprocal lattice

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

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

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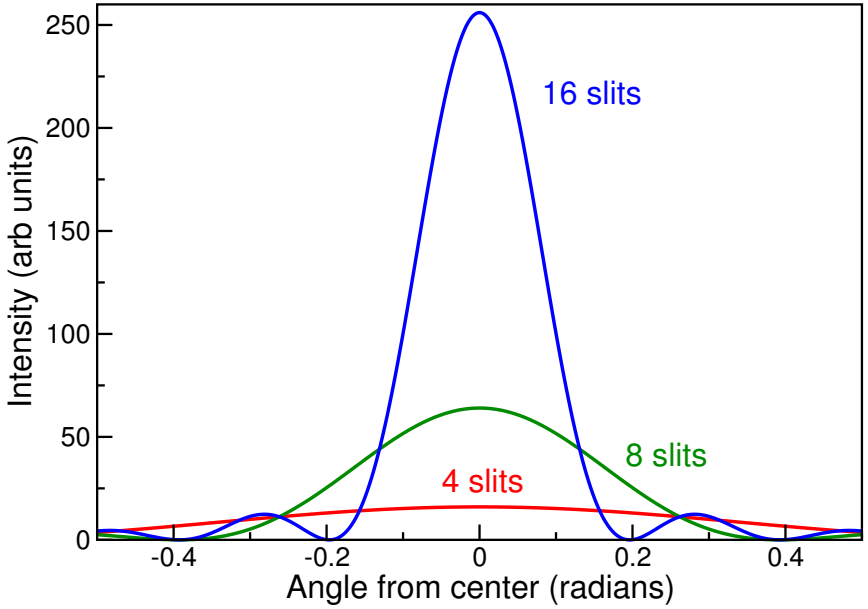

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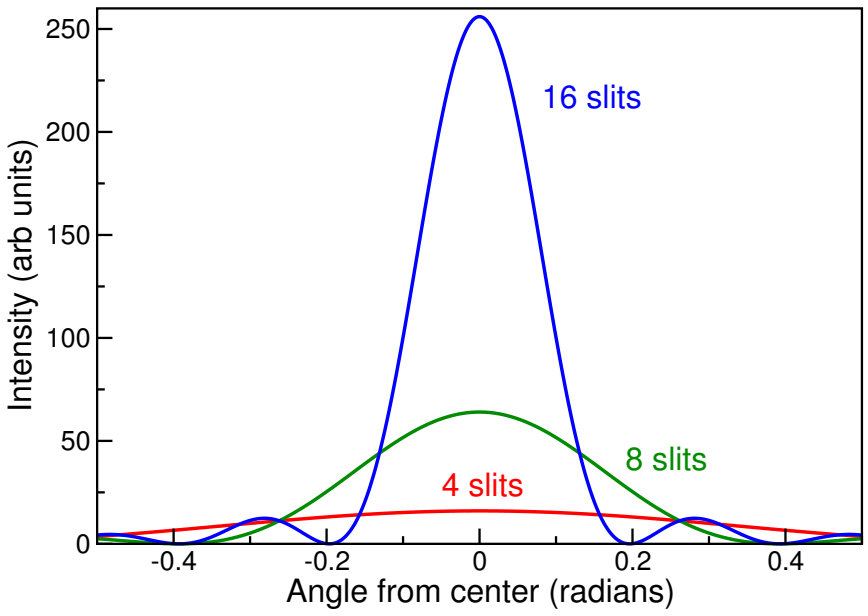

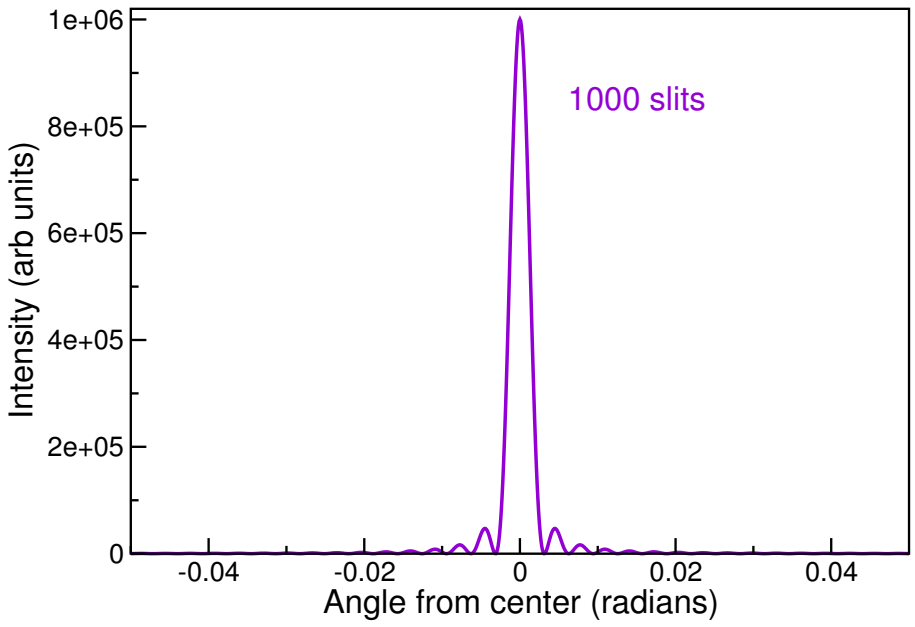

Compton scattering

A photon-electron collision

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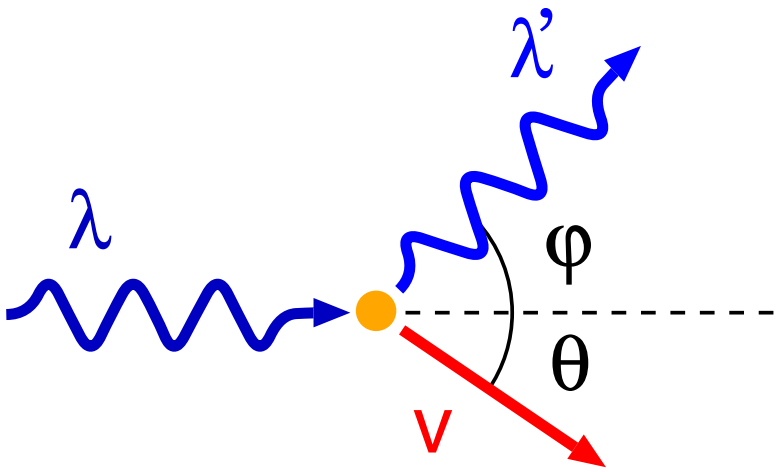

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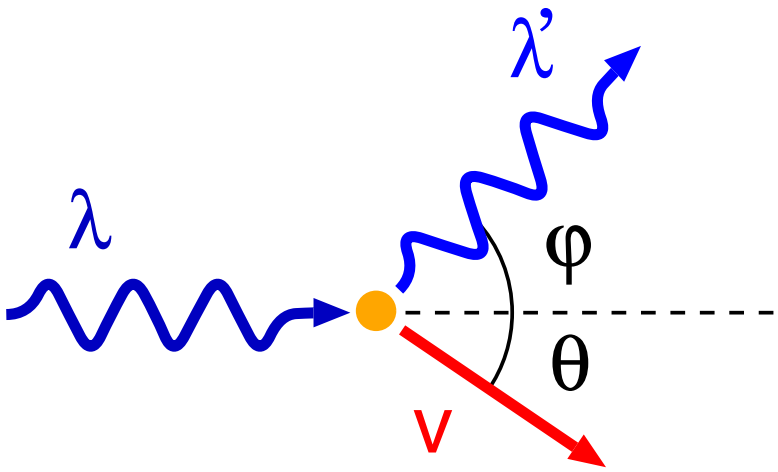

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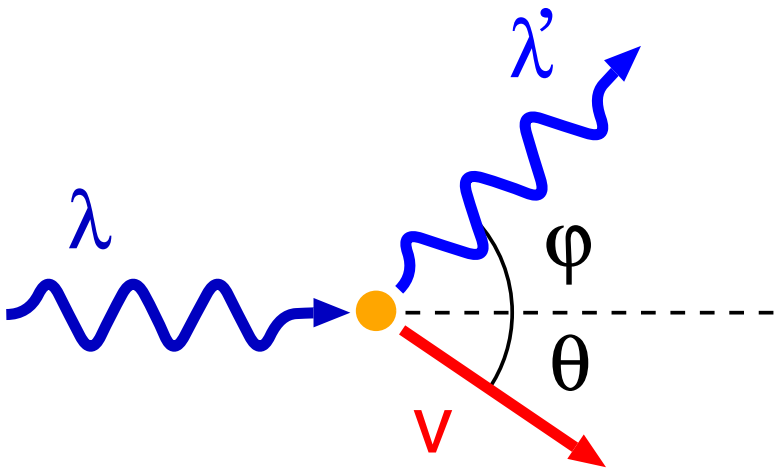

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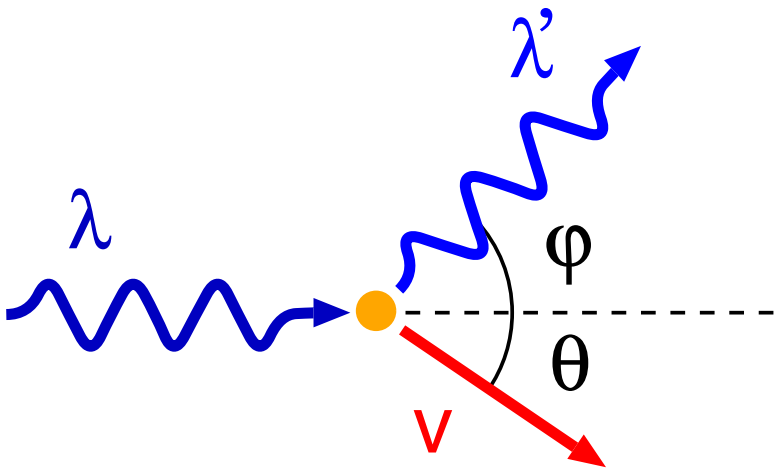

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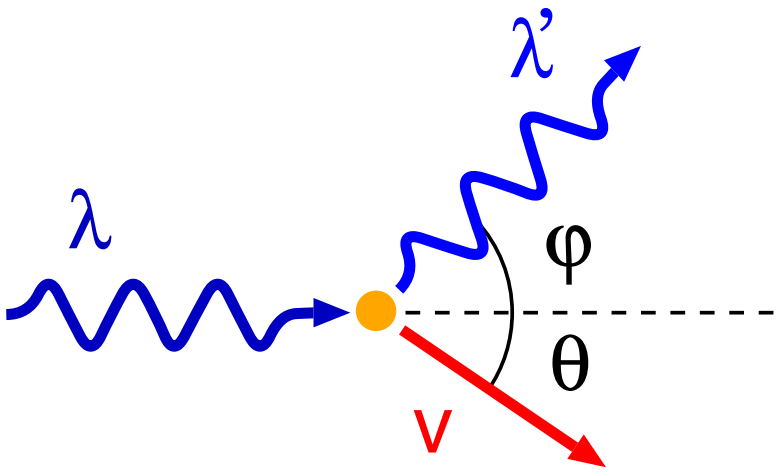

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Treat the electron relativistically and conserve energy and momentum

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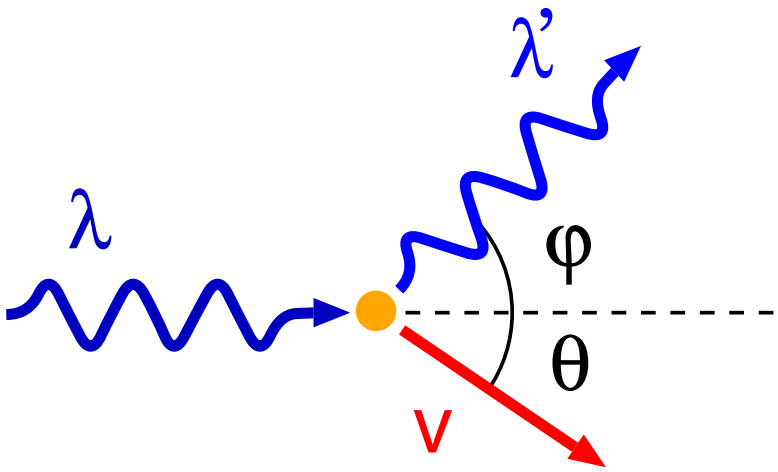

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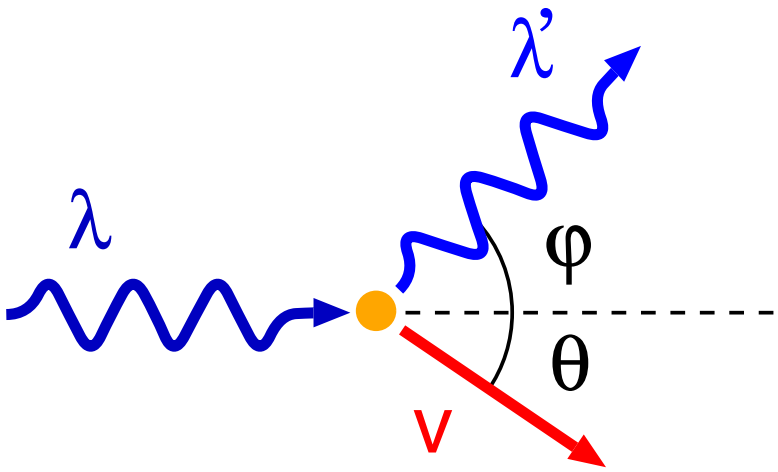

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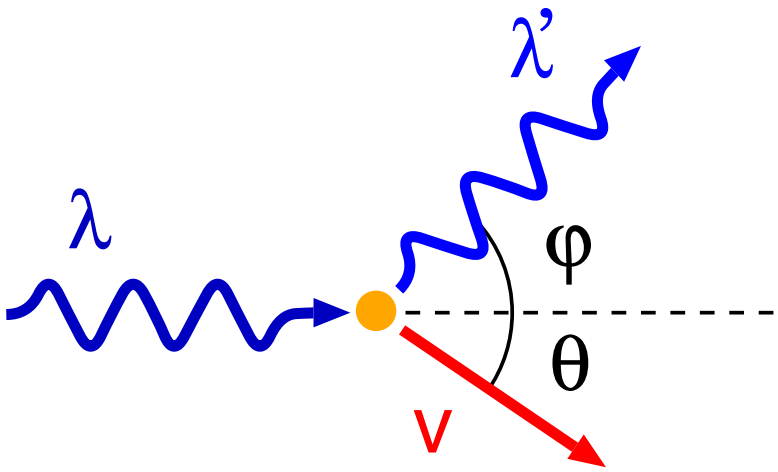

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Compton scattering derivation

squaring the momentum equations

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now add them together,

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

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

Compton scattering derivation

squaring the momentum equations

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Compton scattering derivation

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

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

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Compton scattering derivation

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

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

Compton scattering results

$$\lambda_c = \hbar/mc = 3.86 \times 10^{-3}\text{Å} \text{ for an electron}$$

Comparing to the Thomson scattering length: $r_o/\lambda_C = 1/137$

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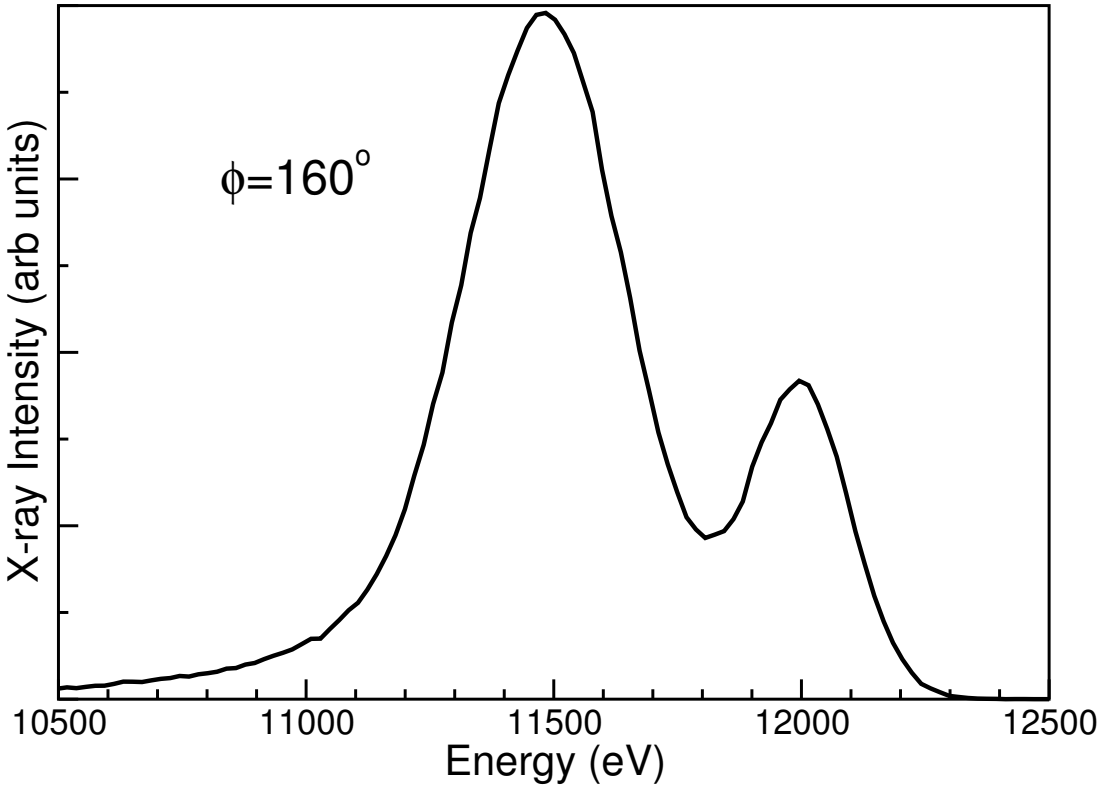
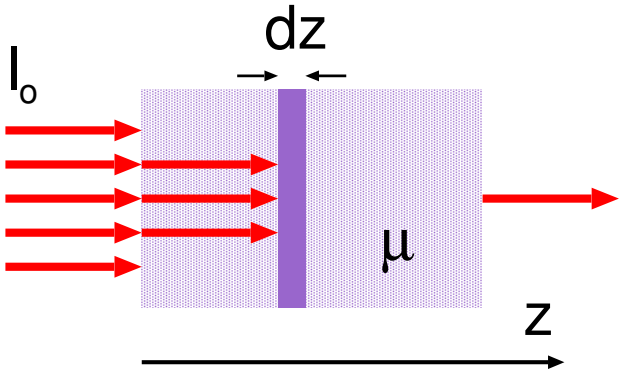


X-ray absorption



Absorption coefficient μ, thickness dz
x-ray intensity is attenuated as

$$dI = -I(z)\mu dz$$

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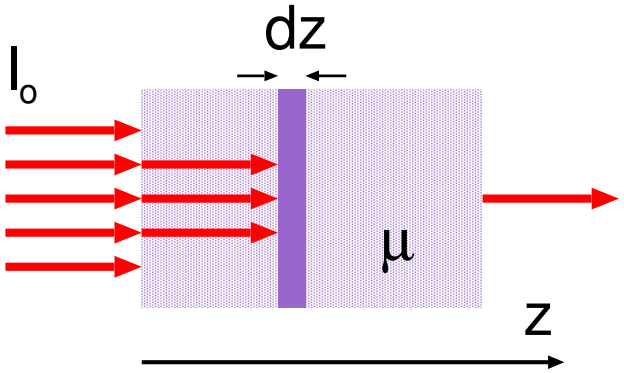

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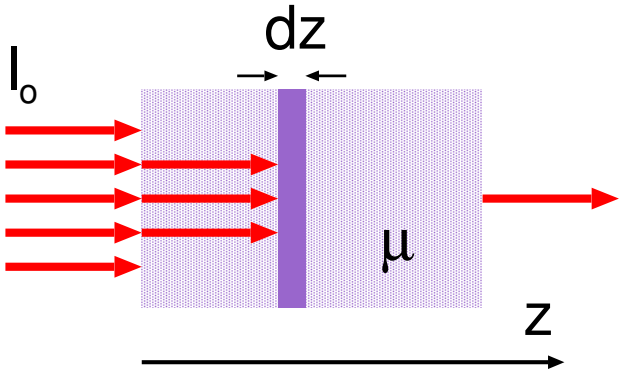

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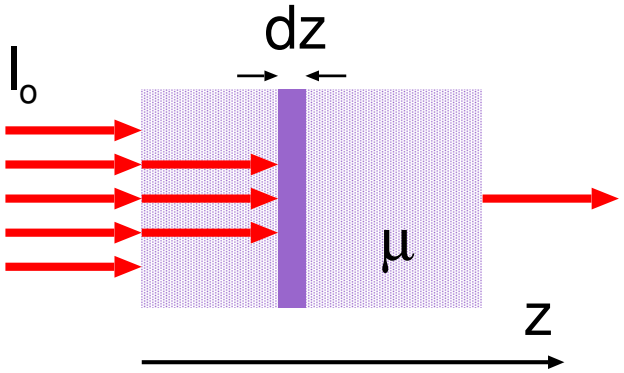

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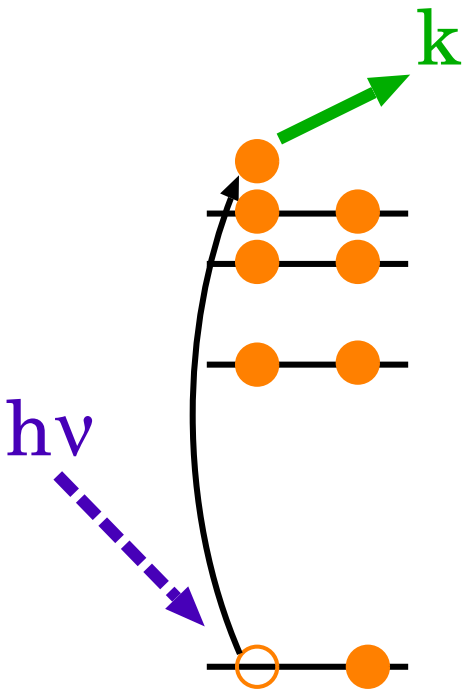
$$\mu = \rho_a\sigma_a = \left(\frac{\rho_m N_A}{A}\right)\sigma_a$$

with mass density ρ_m , Avogadro's number N_A, atomic number A

Absorption event



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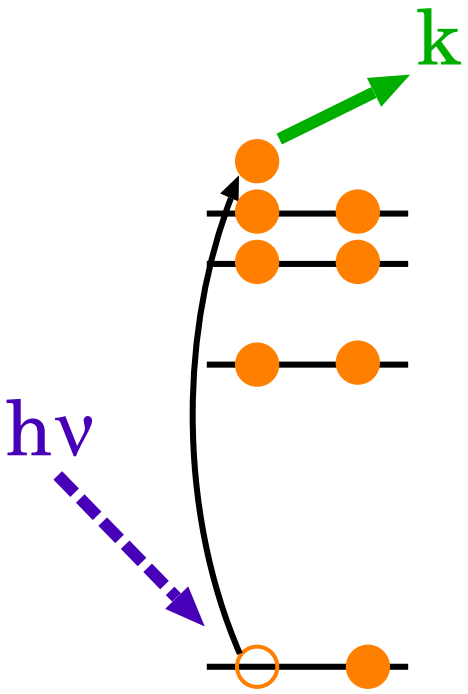
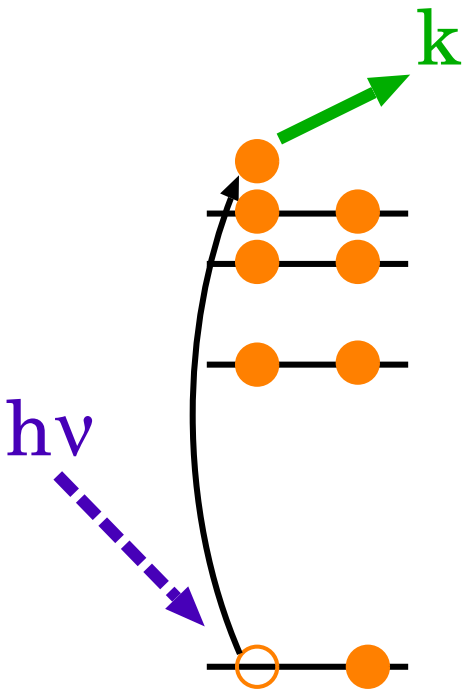


- X-ray is absorbed by an atom
- Energy is transferred to a core electron

Absorption event



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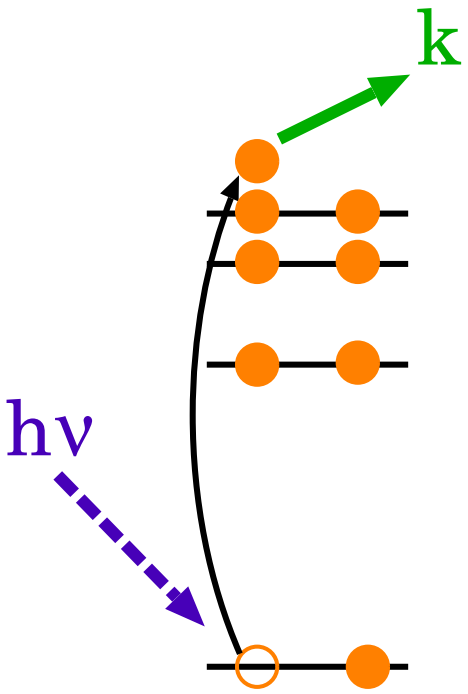

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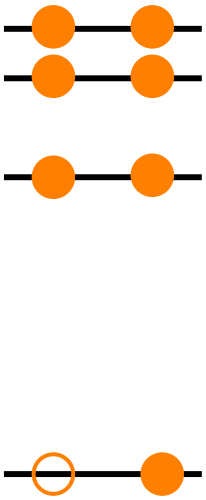
An ion with a core-hole is quite unstable ($\approx 10^{-15}$s)



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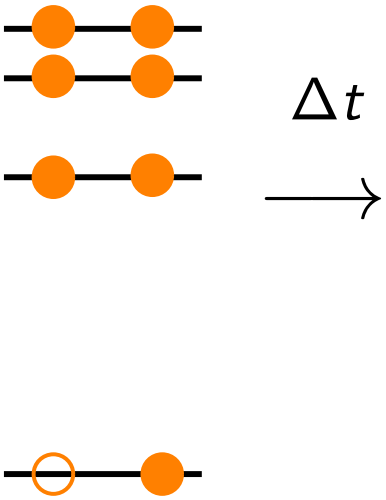

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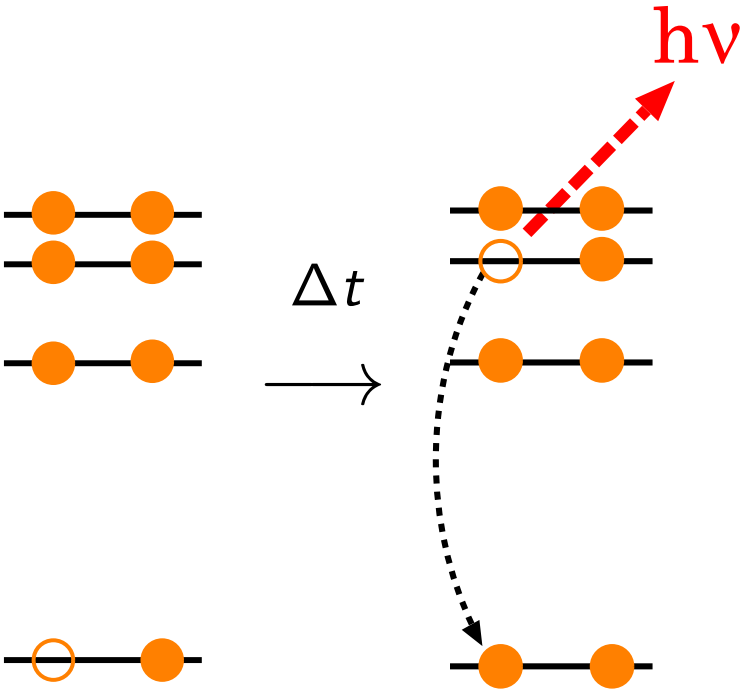

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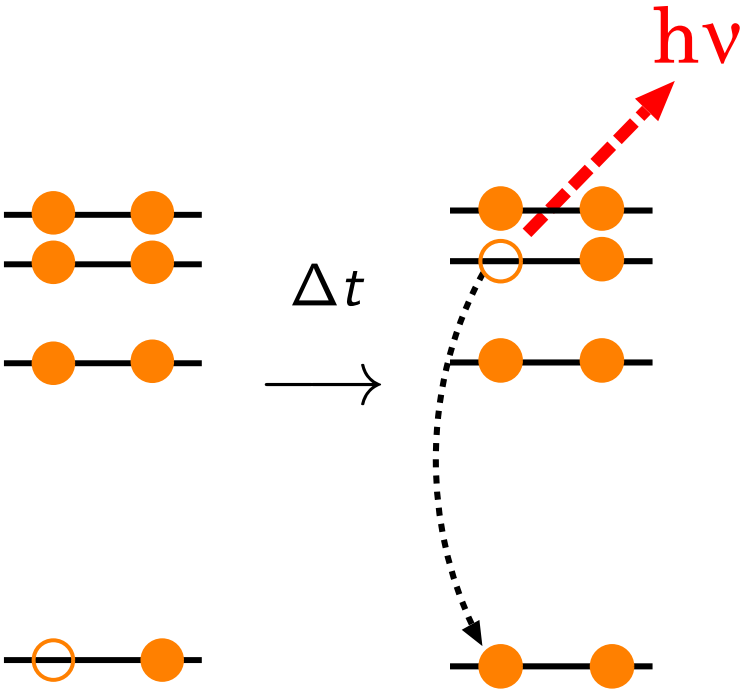

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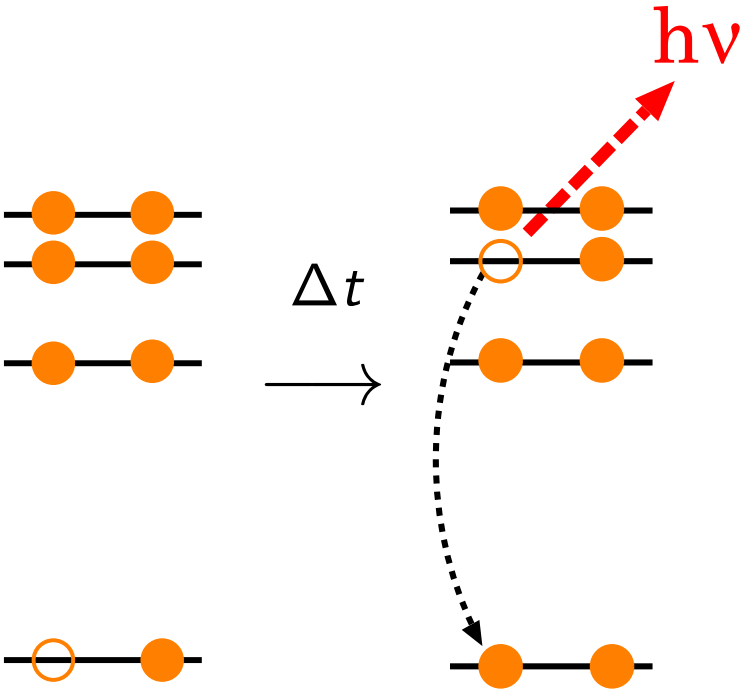

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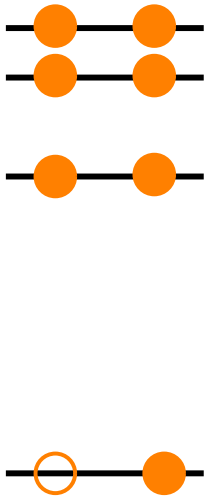
- The result is a cascade of fluorescence photons which are characteristic of the absorbing atom

Auger emission

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



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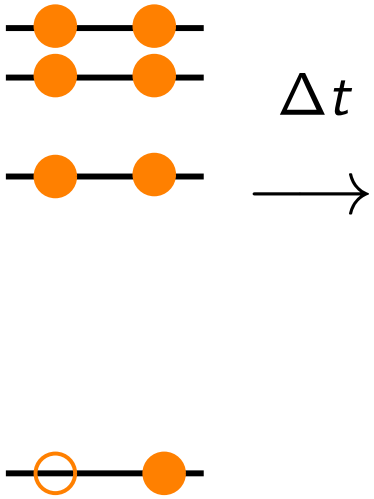

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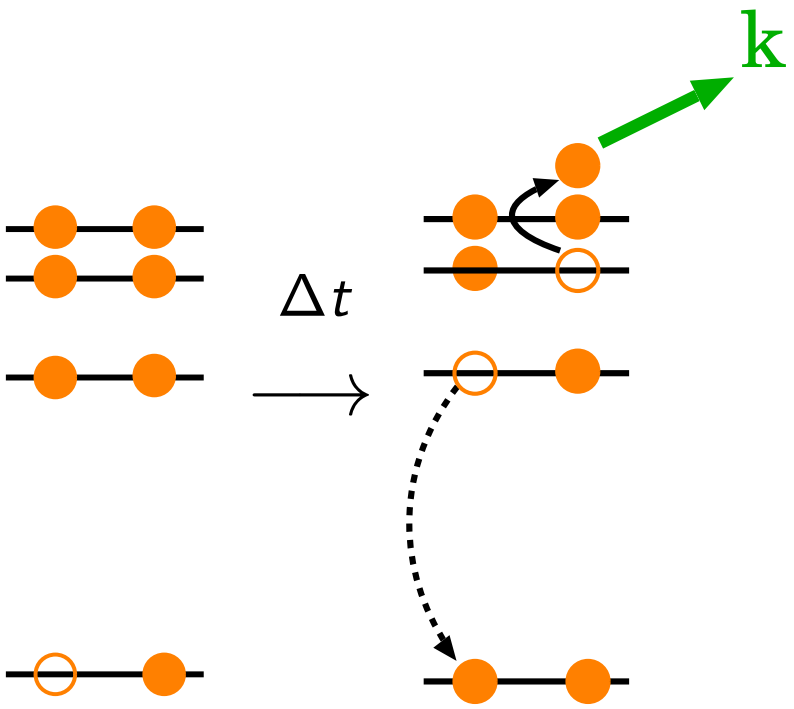

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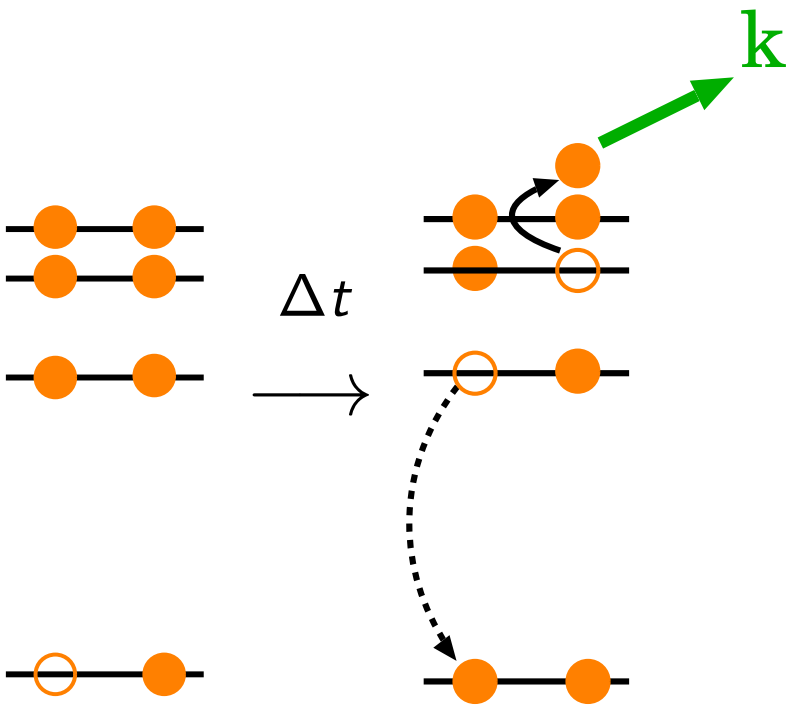

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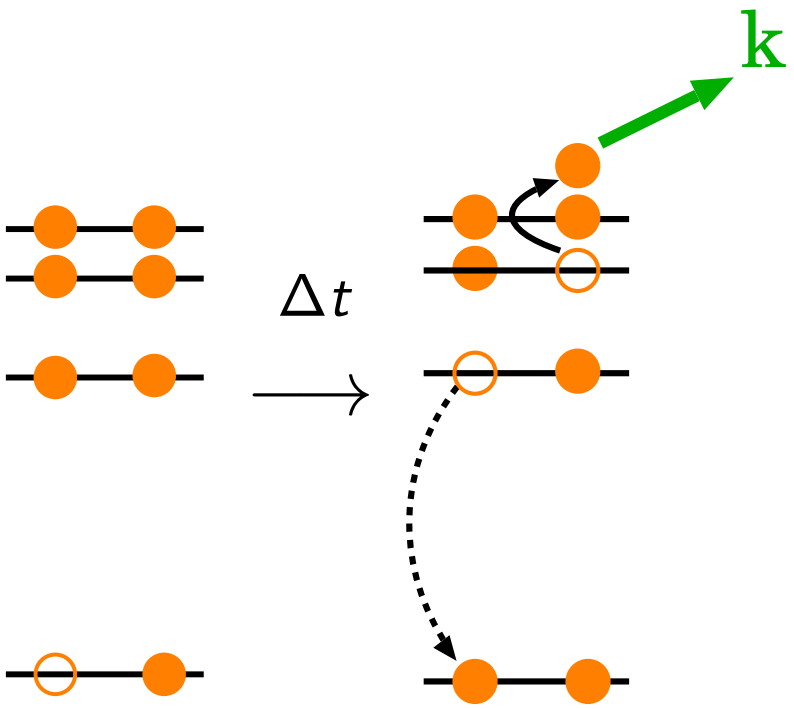

- In the Auger process, a higher level electron will drop down in energy to fill the core hole
- The energy liberated causes the secondary emission of an electron
- This leaves two holes which then filled from higher shells
- So that the secondary electron is accompanied by fluorescence emissions at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

Absorption coefficient

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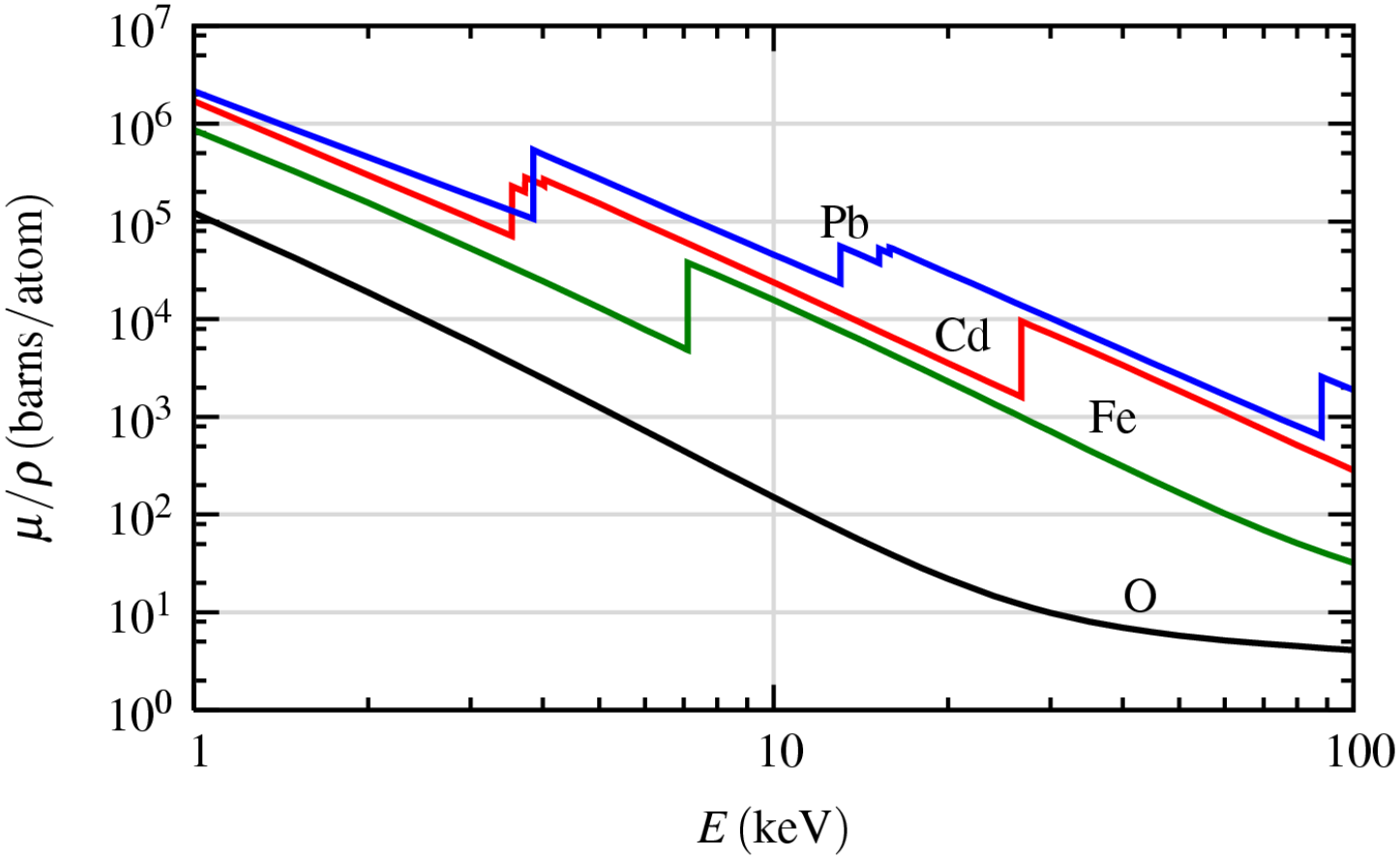
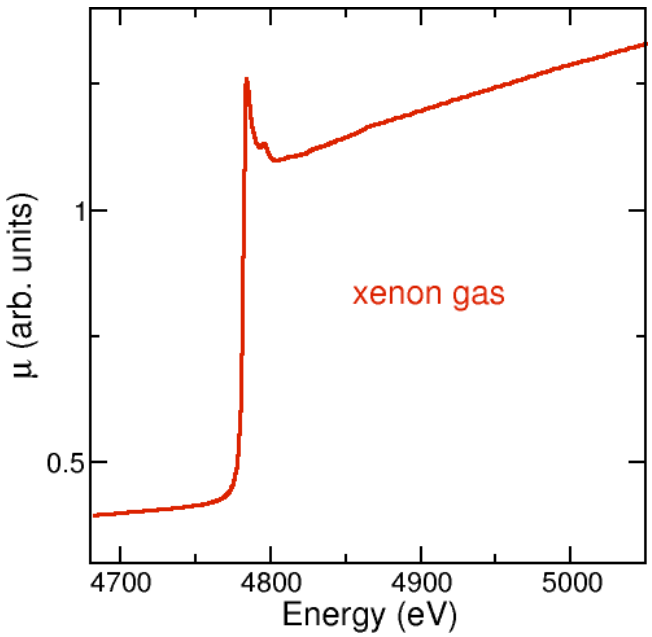


Absorption coefficient

Isolated gas atoms show a sharp jump and a smooth curve



$\longrightarrow$

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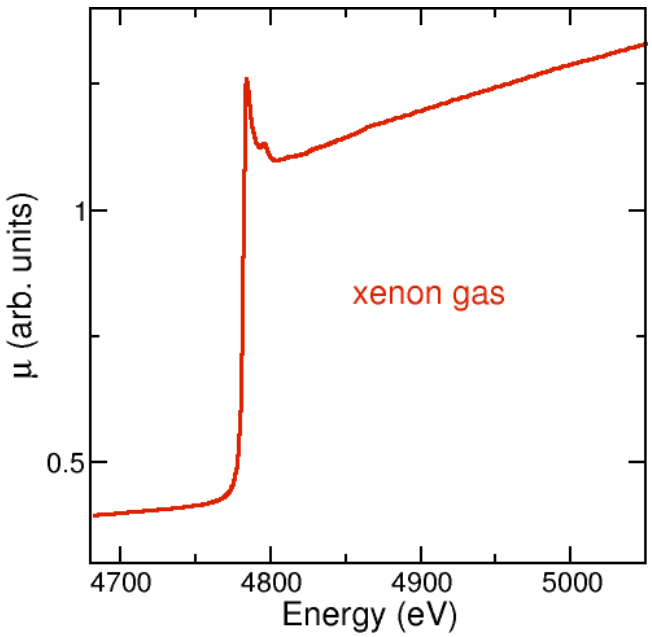
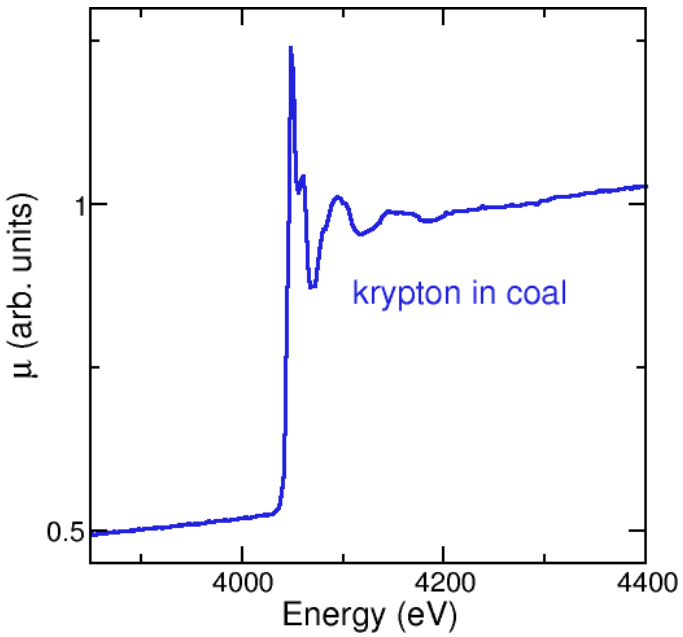
Atoms in a solid or liquid show fine structure after the absorption edge called XANES and EXAFS





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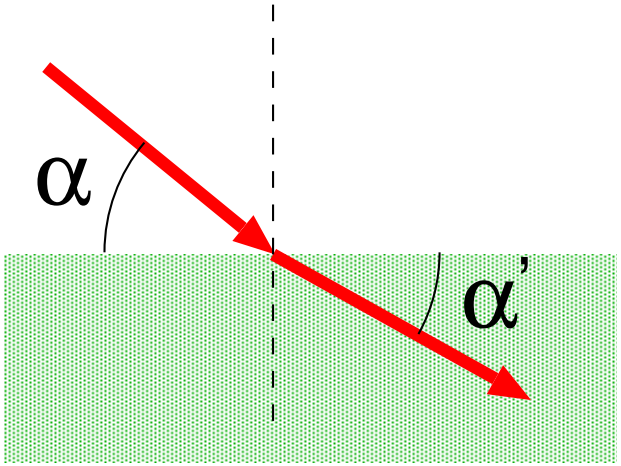

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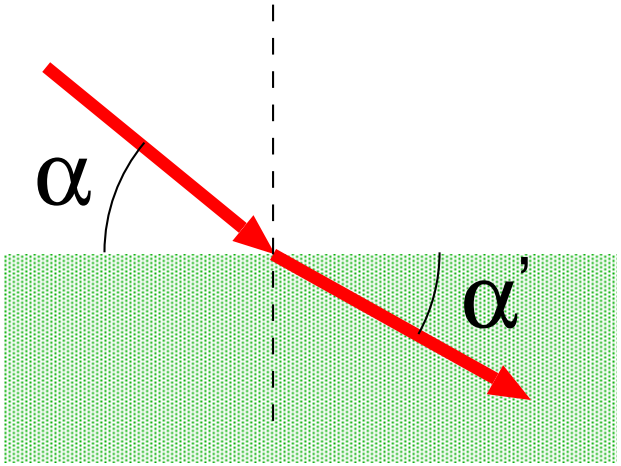

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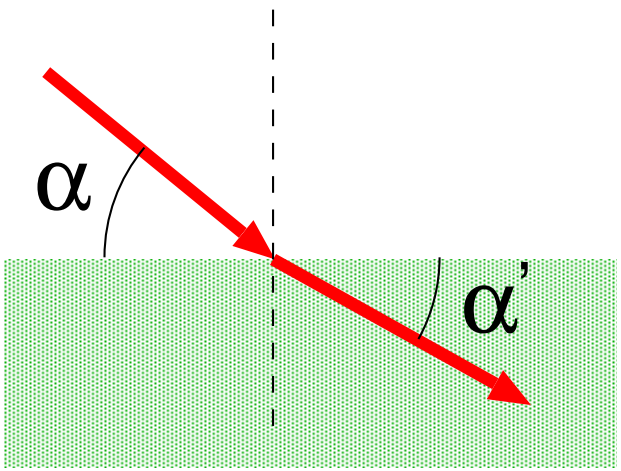

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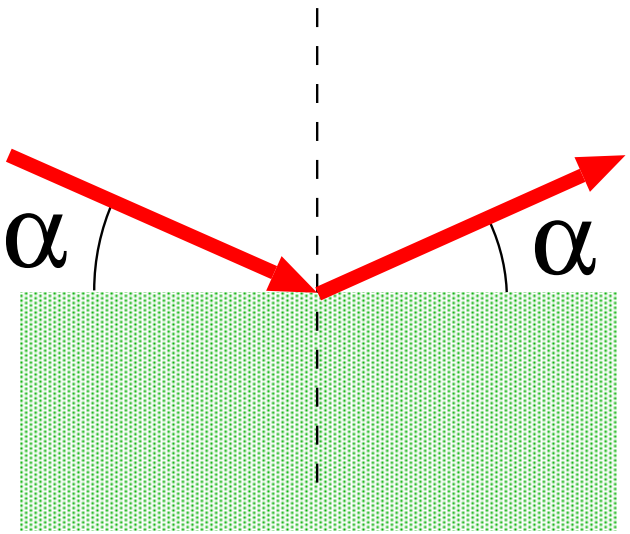

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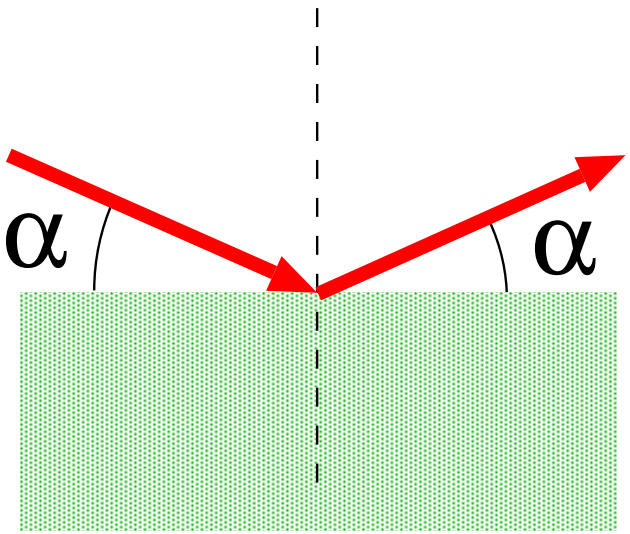

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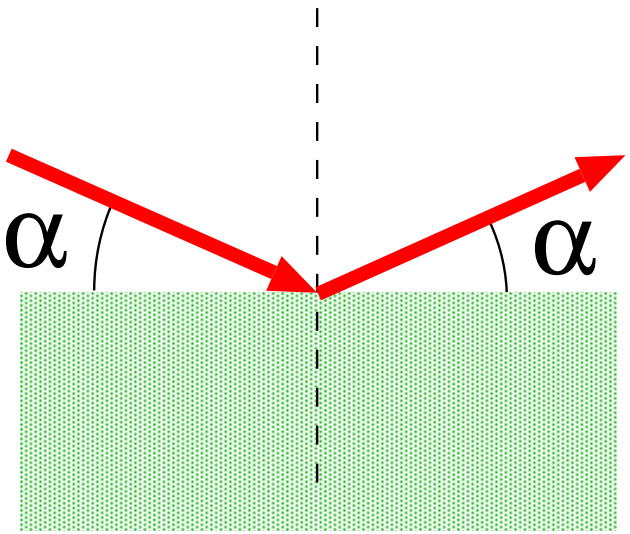

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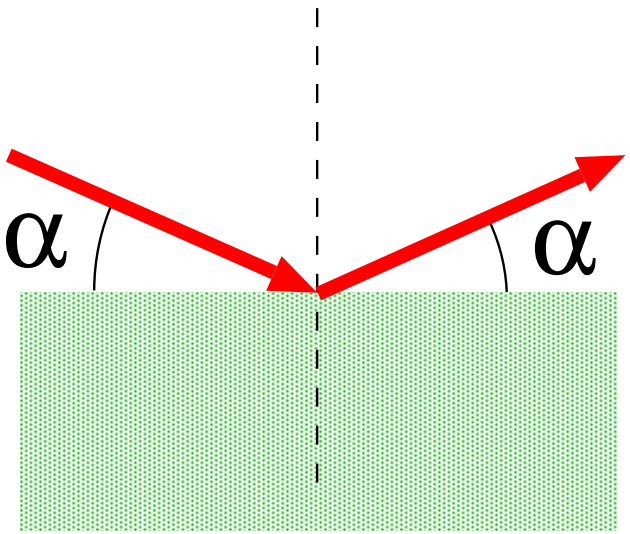

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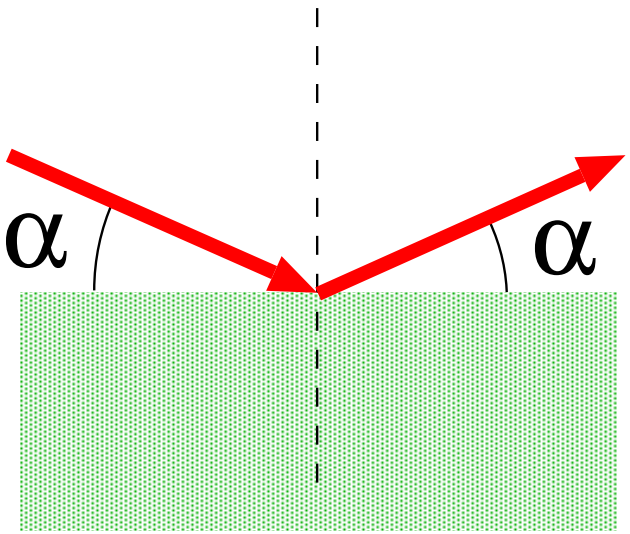

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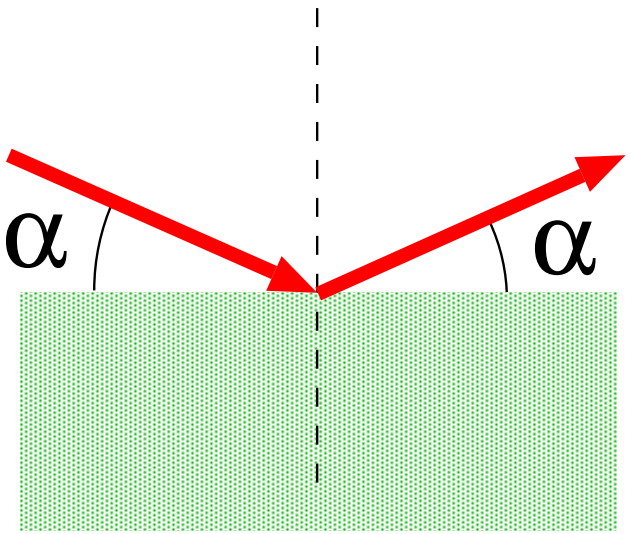

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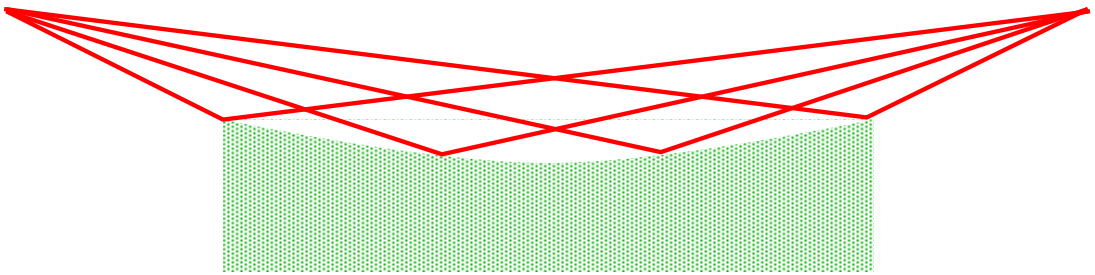
$$\delta = \frac{\alpha_c^2}{2} \quad \longrightarrow \quad \alpha_c = \sqrt{2\delta}$$

Uses of total external reflection



X-ray mirrors

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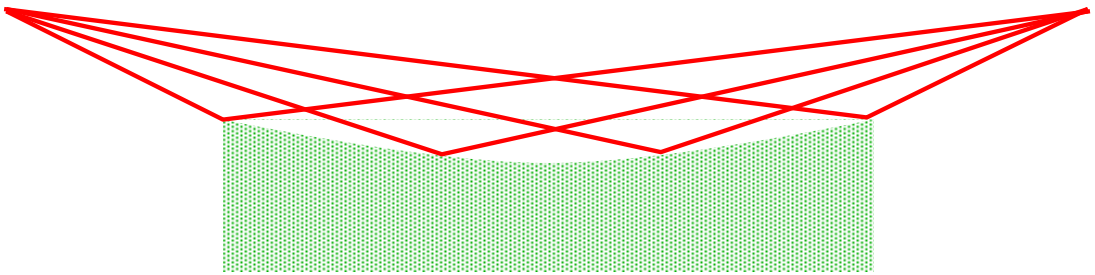

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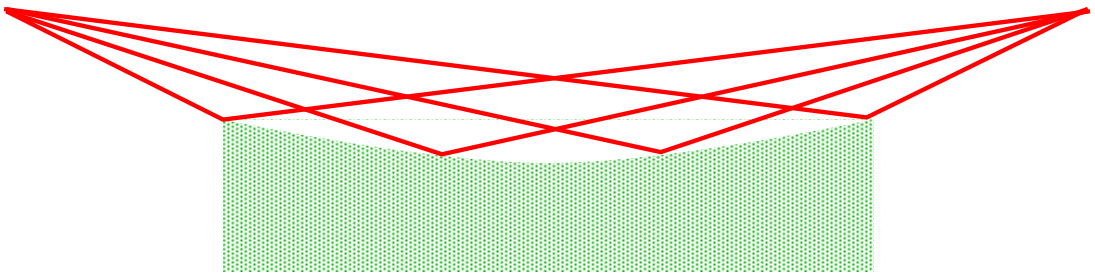

X-ray mirrors

- harmonic rejection
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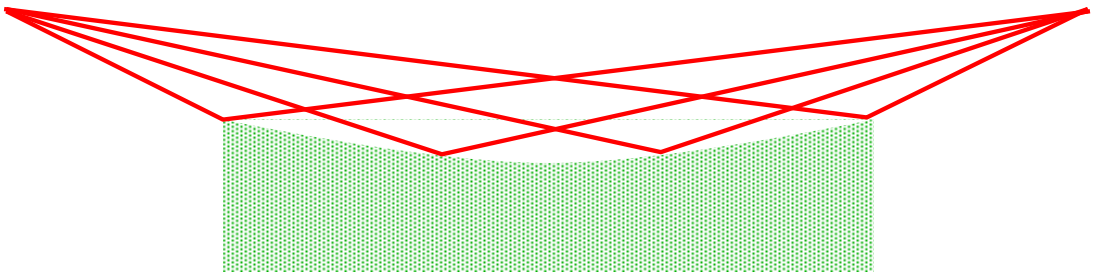

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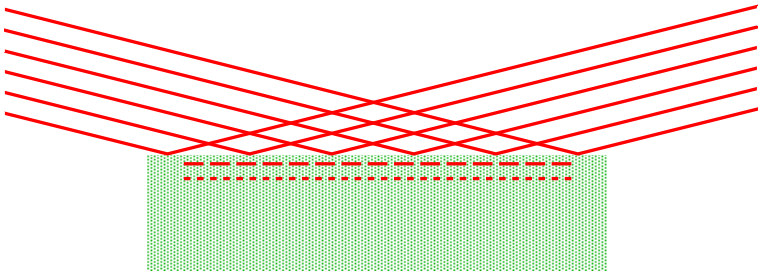

Evanscent wave experiments

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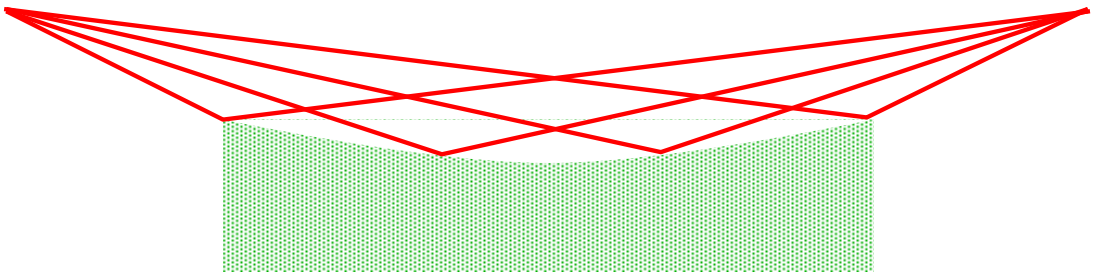

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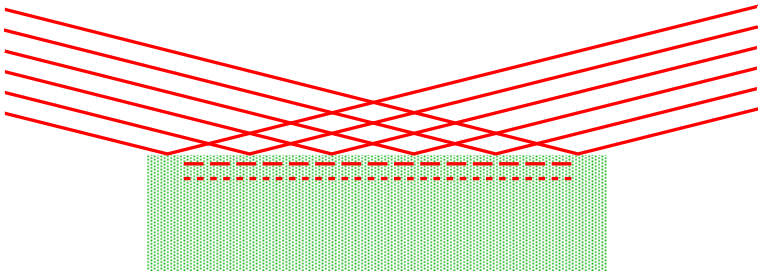

Evanscent wave experiments

- studies of surfaces

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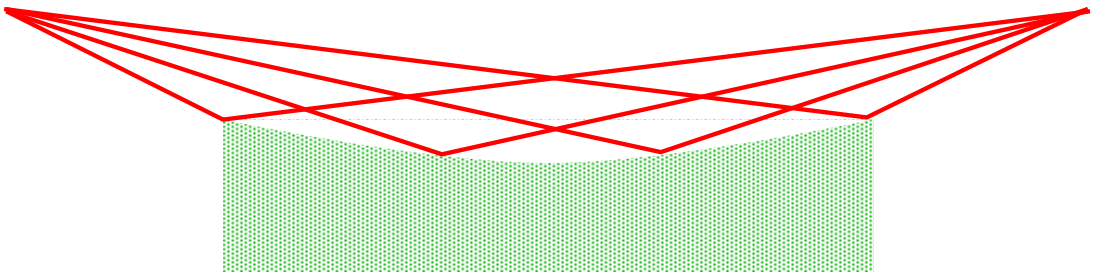

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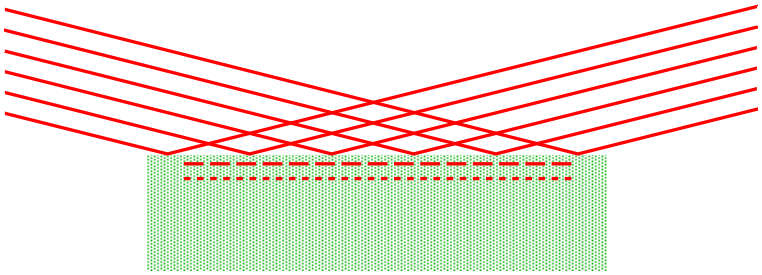

Evanscent wave experiments

- studies of surfaces
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