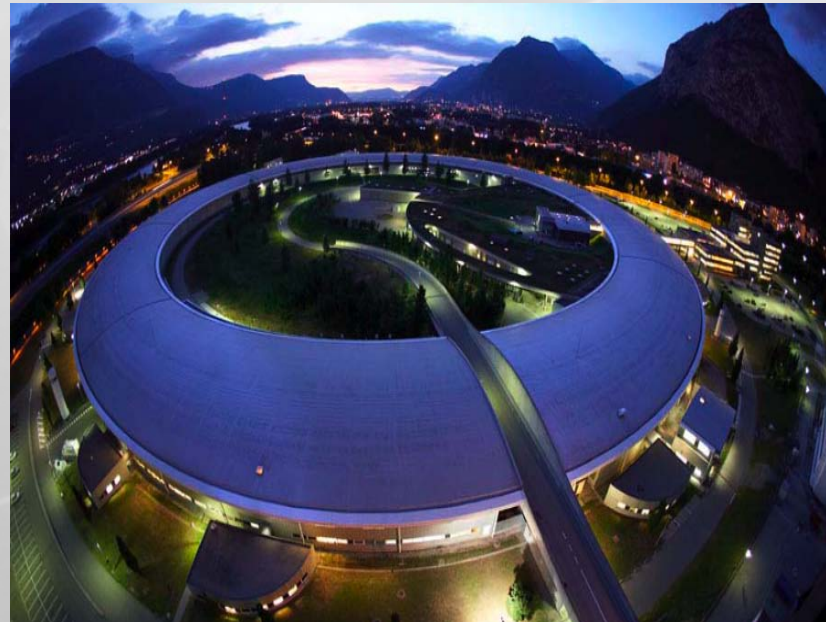


## **“X-rays and their interaction with matter”**



**Luigi Paolasini**

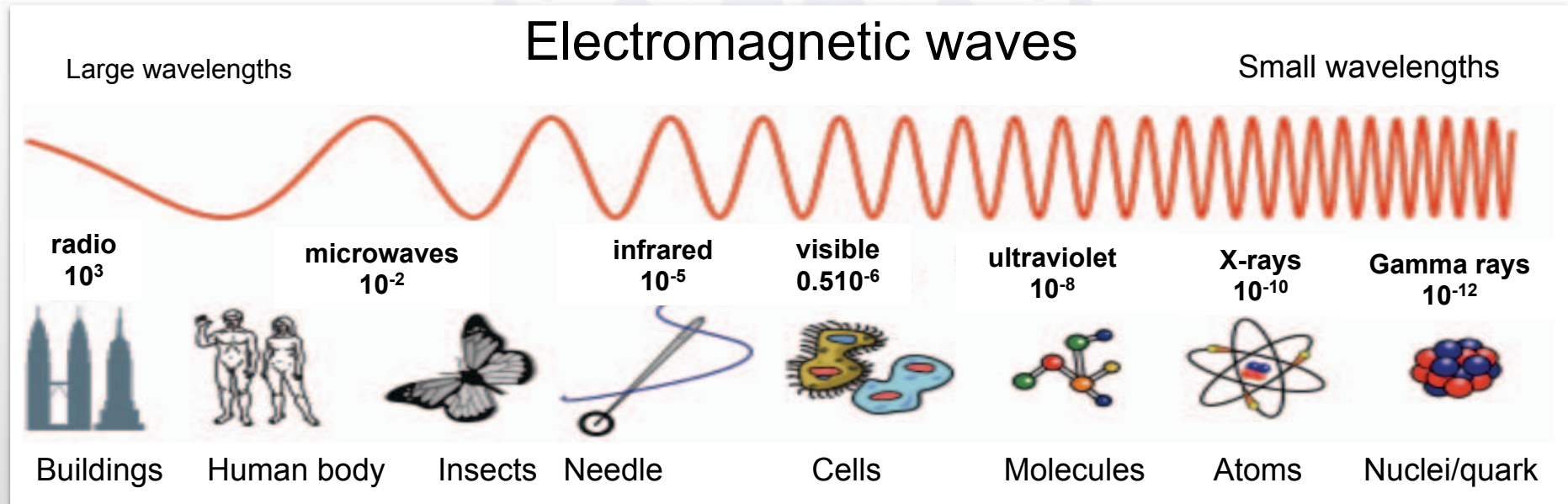
**European Synchrotron Radiation Facility**

**[paolasini@esrf.eu](mailto:paolasini@esrf.eu)**

## **“X-rays and their interaction with matter”**

- 1 – Synchrotron radiation properties
- 2 – Waves and photons
- 3 – Scattering processes
- 4 – Optical properties
- 5 – Absorption

Small wavelength probe small objects



Radio waves



Radar



Microscopes



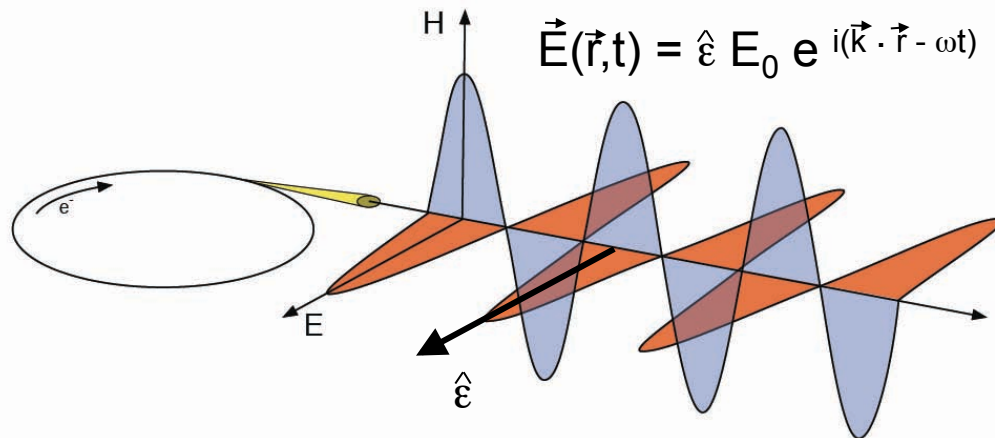
Synchrotrons



Large accelerators

The synchrotron radiation delivered by insertion devices is a polarized electromagnetic wave with polarization vector  $\hat{\varepsilon}$  parallel to the electric field  $E$  and lying in the synchrotron orbit plane.

## Transverse EM waves



$$\vec{E}(\vec{r}, t) = \hat{\varepsilon} E_0 e^{i(\vec{k} \cdot \vec{r} - \omega t)}$$

$\lambda$  wavelength

$k=2\pi/\lambda$  wavenumber

$\nu=\omega/2\pi$  frequency

$\hat{\varepsilon}$  polarization

## Energy

$$\hbar\omega = hc/\lambda = 12.398 \text{ [keV]} / \lambda \text{ [\AA]}$$

$$\lambda \text{ [\AA]} = hc/\hbar\omega = 12.398/E[\text{keV}]$$

$$\text{ex. } 1 \text{ \AA} = 12.398 \text{ keV}$$

## Spectral intensity

$$I_0(\omega) = \langle E_0^2 \rangle = N(\omega) \hbar\omega$$

## High brilliance

- Easy focusing, fast detection

## Short Wavelengths

- Comparable with atomic distances

## Energy resolution and tuning

- Core-hole electron transitions energies

## Polarization

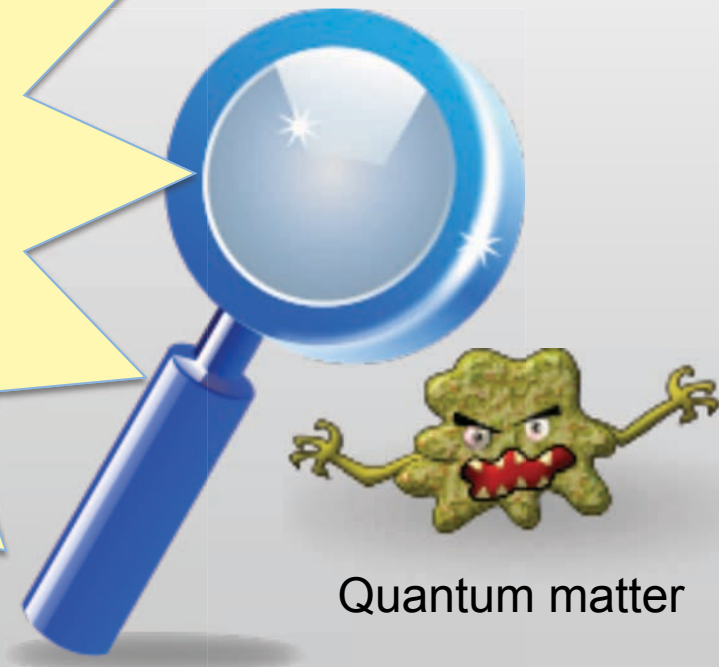
- Magnetic and electronic symmetries

## Time structure

- Pump probe experiments

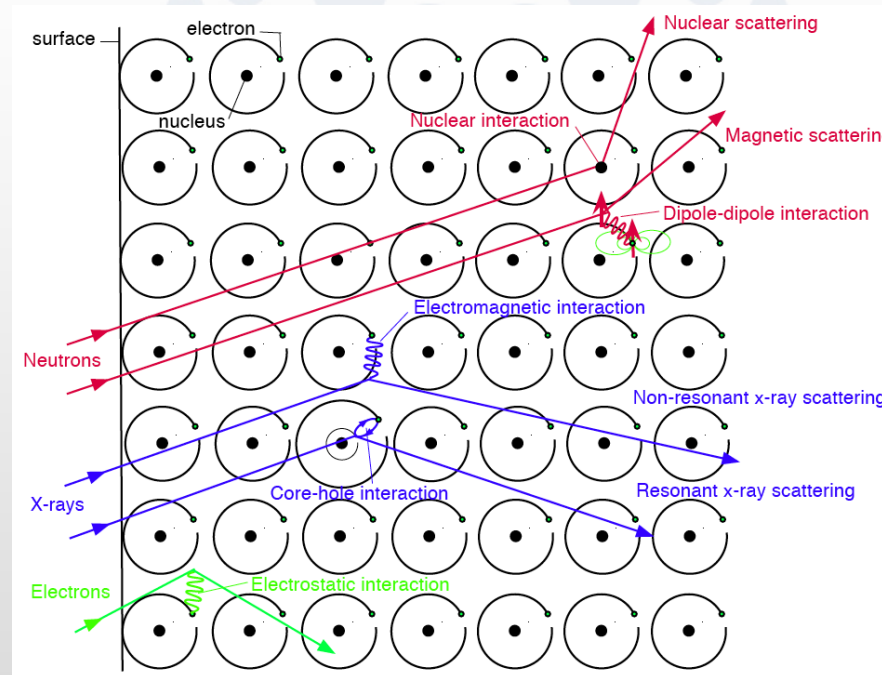
## Coherence

- Photon correlation spectroscopies



Quantum matter

Neutron and x-ray magnetic scattering are a powerful probe to study the electronic interactions at atomic scale in bulk and nanostructured materials

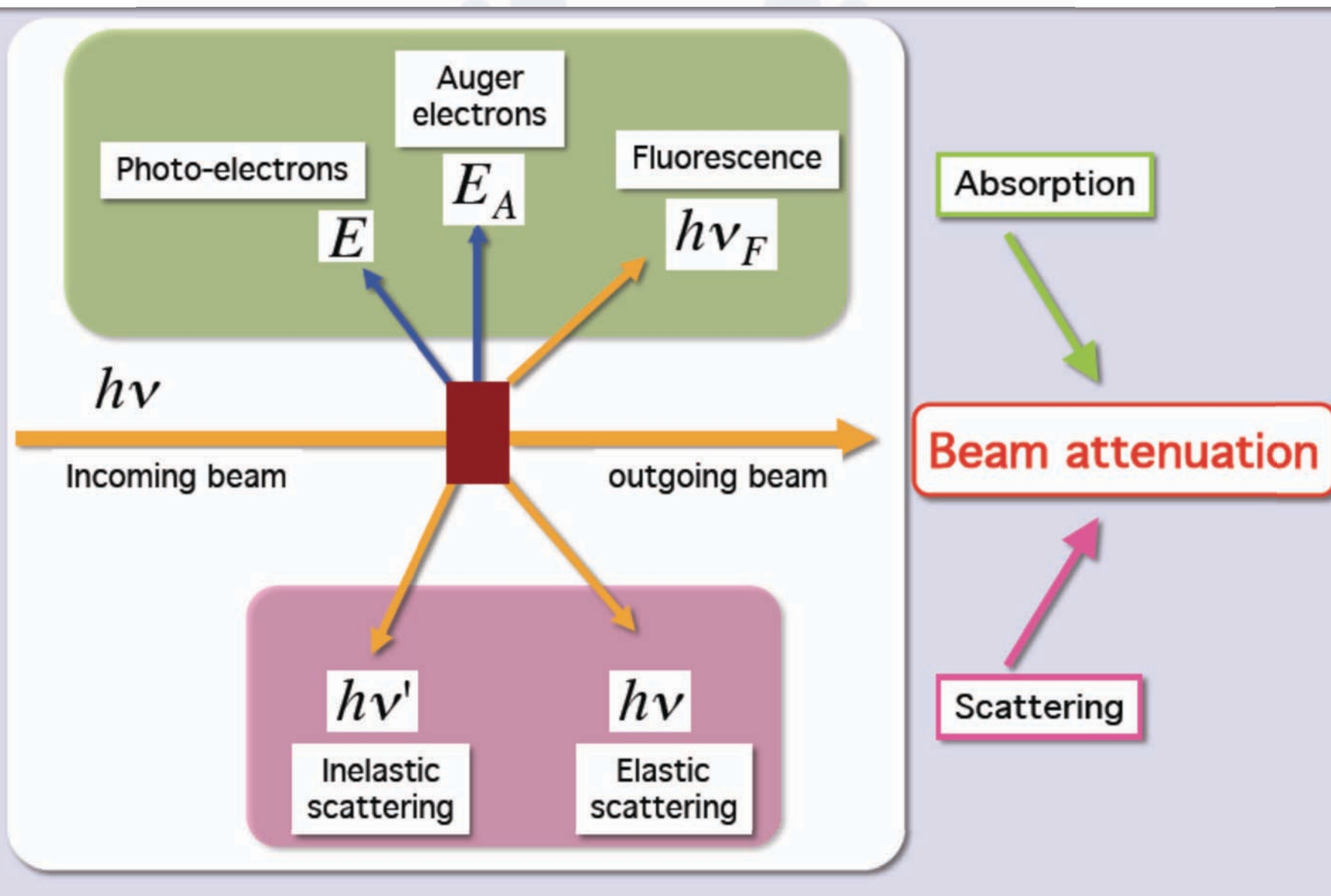


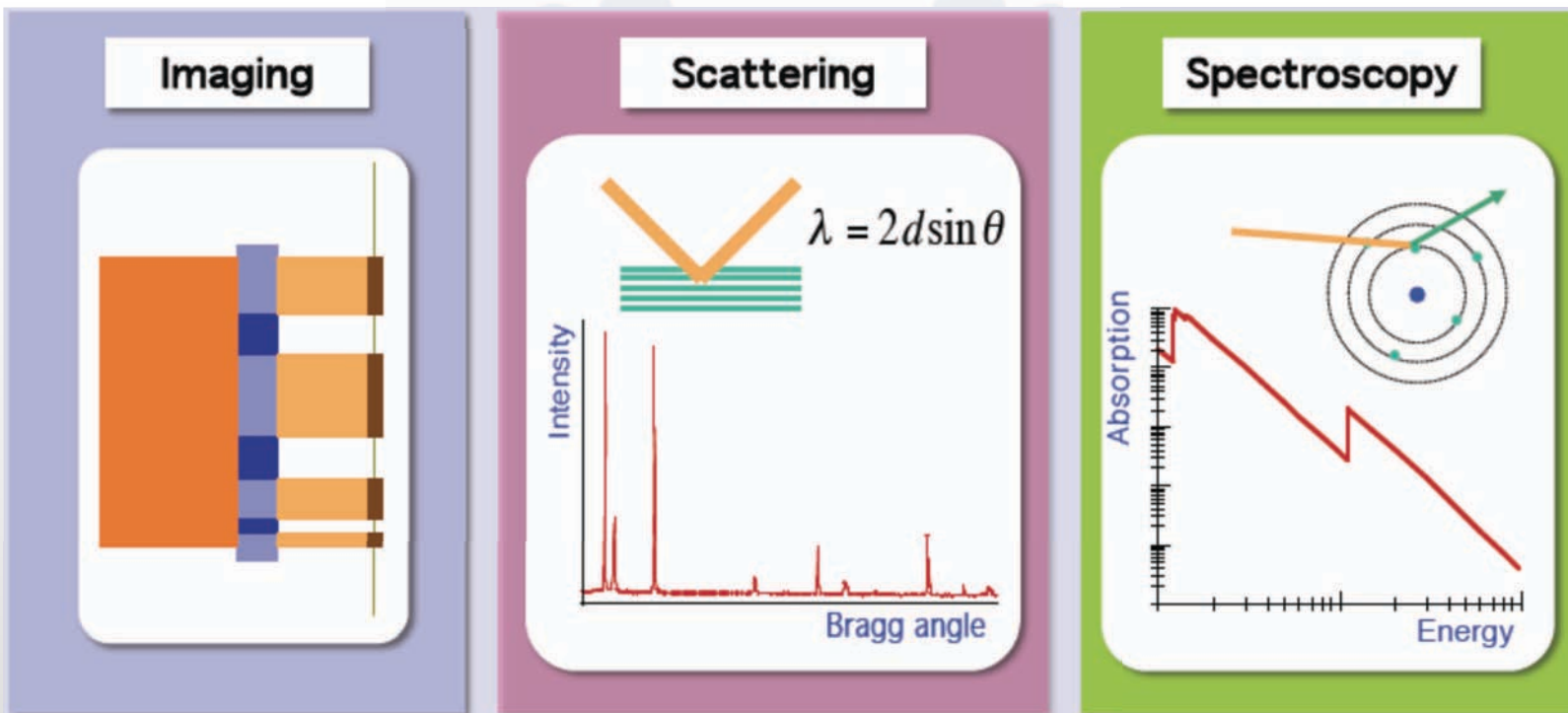
## Neutron scattering (Cold-Thermal)

- Bulk sensitivity (low absorp., ~10 cm)
- Amplitudes: Nuclear/Magnetic ~ 1
- High E-resolution
- **Unpolarized source**
- Soft interaction neutron-sample
- Well established sample environment

## X-ray scattering (3-30 keV)

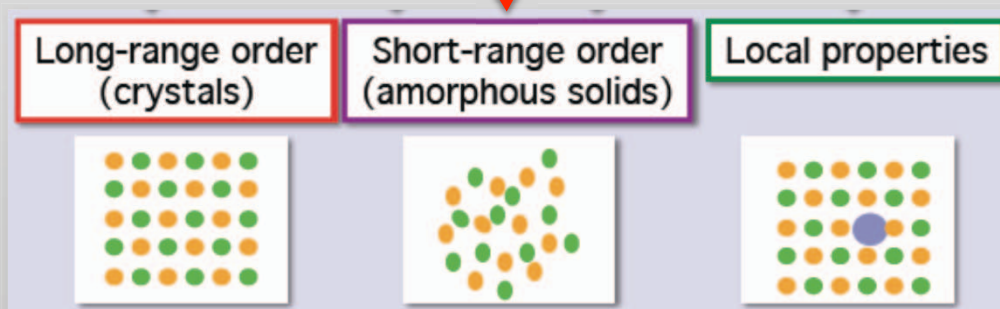
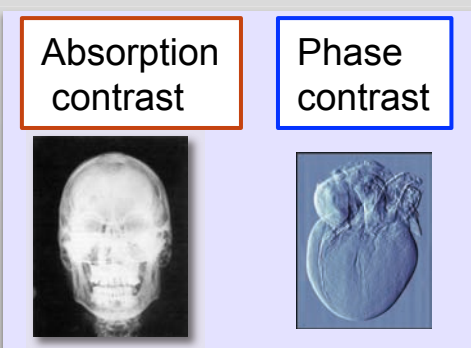
- Surface sensitivity (high absorp., ~10  $\mu\text{m}$ )
- Amplitudes: Charge/Magnetic ~  $10^5$
- High Q-resolution
- **Polarized source**
- **Easy Focusing**
- Hard probe (T-heating, sample damage)...





Spatial informations

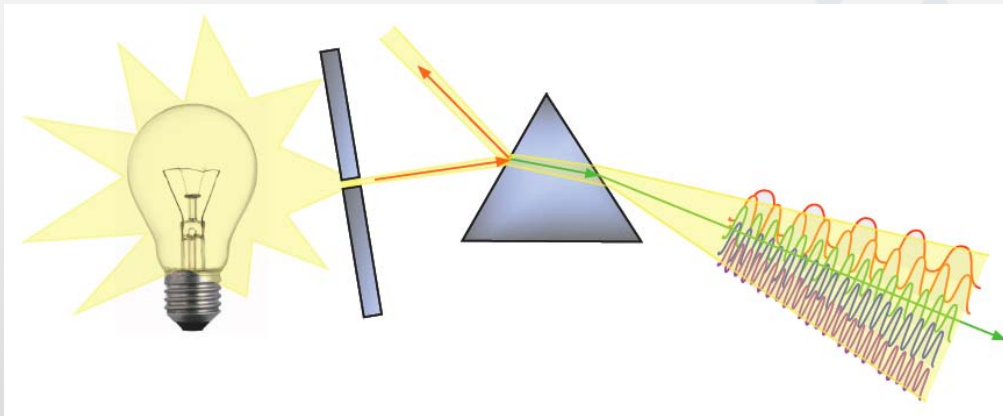
Structural informations





## Electromagnetic waves

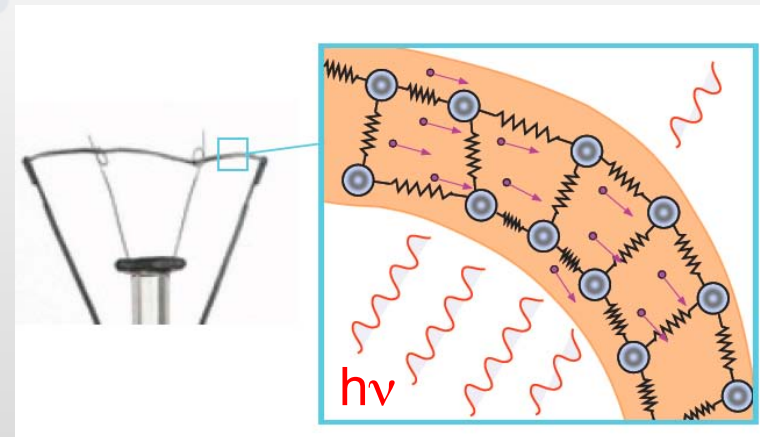
Far from the emission sources  
 Large length scales and forces strengths  
 Classical electromagnetism



- Maxwell equations
- Optics laws:
  - Reflection
  - Refraction
  - Diffraction

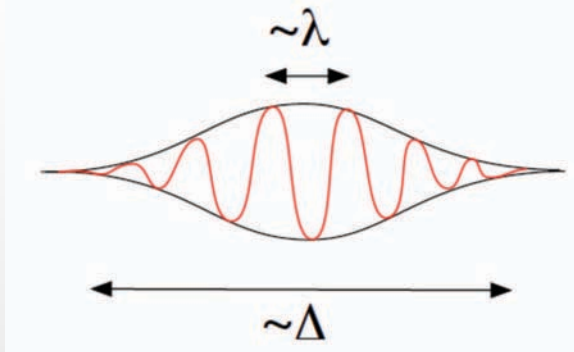
## Photons

Near the emission sources  
 Atomic length scales  
 Quantum mechanics



- Plank laws
- Quantum electrodynamics
- Absorption/emission processes
- Elastic and inelastic scattering

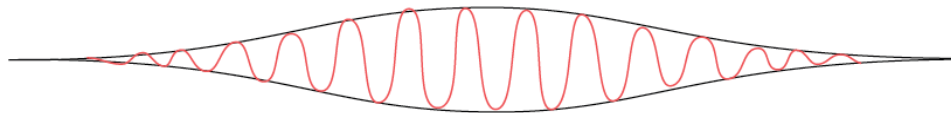
## Matter wave



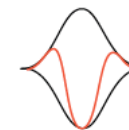
Heisenberg uncertainty principle:  
Cannot define both  $\Delta$  and  $\lambda$  to an arbitrary accuracy

Oscillations → wave  
Envelope → particle

Classical:  $\Delta \gg \lambda$



Quantum:  $\Delta \ll \lambda$



Decreasing  $\Delta$  to define better the position, but we lose information on  $\lambda$

## Kinematics

Energy:  $E = h\nu = \hbar\omega$

Momentum:  $p = h/\lambda = \hbar k$

where

$h$  = Planck's constant

$\nu$  = frequency

$k$  = wavevector

## Assumption of quantum mechanics:

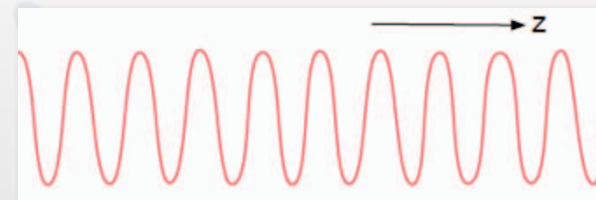
- (i) Particle is represented mathematically by a wavefunction,  $\psi(\underline{r})$
- (ii) Probability of finding a particle in a (infinitesimal) volume  $dV$  is  $|\psi(\underline{r})|^2 dV$

### Infinite plane wave:

$$\psi(z) = e^{ikz} = \cos(kz) + i \sin(kz)$$

$$|\psi|^2 = \psi\psi^* = e^{ikz}e^{-ikz} = 1$$

1 particle per unit volume everywhere!

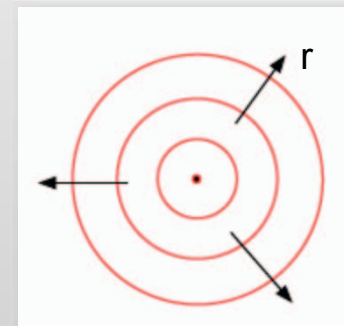


### Spherical wave:

$$\psi(\underline{r}) = b/r e^{ikr}$$

$$|\psi(\underline{r})|^2 = b^2/r^2$$

Density of particles falls as  $1/r^2$



### Flux of particles

$$\begin{aligned} I &= \text{No. of particles incident normally on unit area per second} = \\ &= \text{particle density} \times \text{velocity} \\ &= |\psi|^2 \times v = |\psi|^2 \hbar k/m \quad (\text{m}^{-2} \text{s}^{-1}) \end{aligned}$$

## Definition: Total cross section

$$\sigma = \frac{\text{Total no. particles scattered in all the directions per second}}{\text{Incident flux } (I_0)}$$

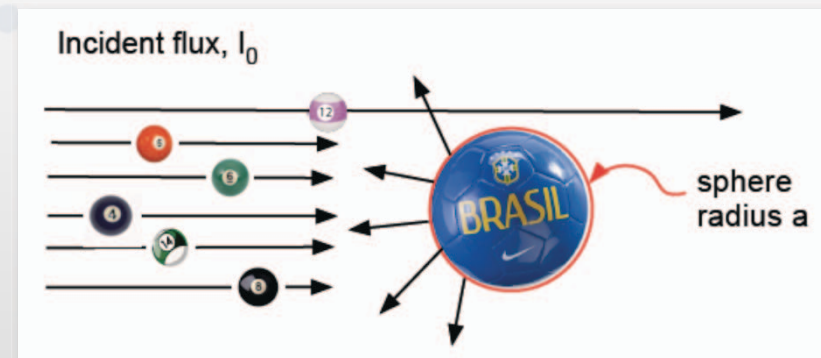
## Classical case:

$$\text{no. particles scattered per second} = I_0 \times \pi a^2$$

$$\sigma = \pi a^2$$

Particles per unit area per sec.

Cross-sectional area of sphere



## Quantum case:

Incident wave

$$\psi_0 = e^{ikz}$$

Incident flux

$$I_0 = |\psi_0|^2 v = v$$

Scattered wave

$$\psi_{sc} = \frac{b}{r} e^{ikr}$$

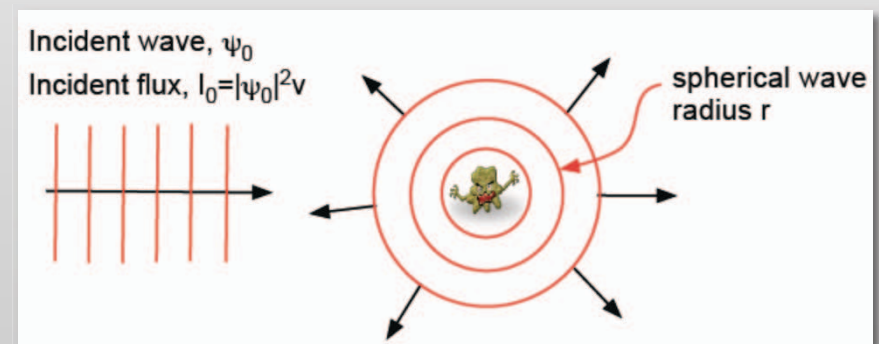
Scattered flux

$$I_{sc} = |\psi_{sc}|^2 v = \frac{b^2 v}{r^2}$$

$$\text{no. particles scattered per second} = I_{sc} \times 4\pi r^2$$

$$\sigma = 4\pi b^2$$

Effective area viewed by scattering particles!  
b is the scattering amplitude



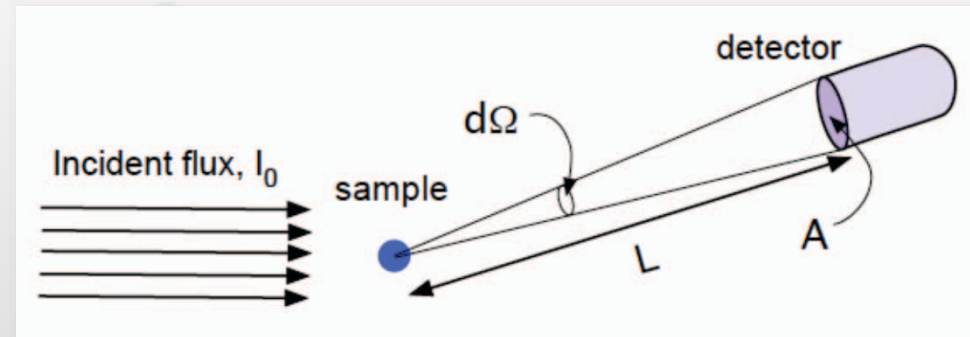
## Definition: differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{\text{no. particles scattered into solid angle } d\Omega \text{ per sec.}}{I_0 \times d\Omega}$$

Solid angle subtended by detector:  
 $\Delta\Omega = A/L^2$

No. particles detected per sec.:  
 $I_0 \Delta\Omega \frac{d\sigma}{d\Omega} = |\psi_{sc}|^2 v \times A$

$\swarrow$  Flux                       $\searrow$  Detector area



$$\frac{d\sigma}{d\Omega} = \frac{|\psi_{sc}|^2}{|\psi_0|^2} L^2 = b^2 = \frac{d\sigma}{4\pi}$$

(barns/steradian)

1 barn =  $10^{-28} \text{ m}^2$

Notice that  $\psi_{sc}$  is a spherical wave  $|\psi_{sc}|^2 = b^2/L^2$

- ◆ The electric field  $E_{in}$  of the incident x-rays forces the motion of the electron which radiates a spherical wave  $E_{rad}$ .
- ◆ Electron at rest: Electric Force  $F=Eq$

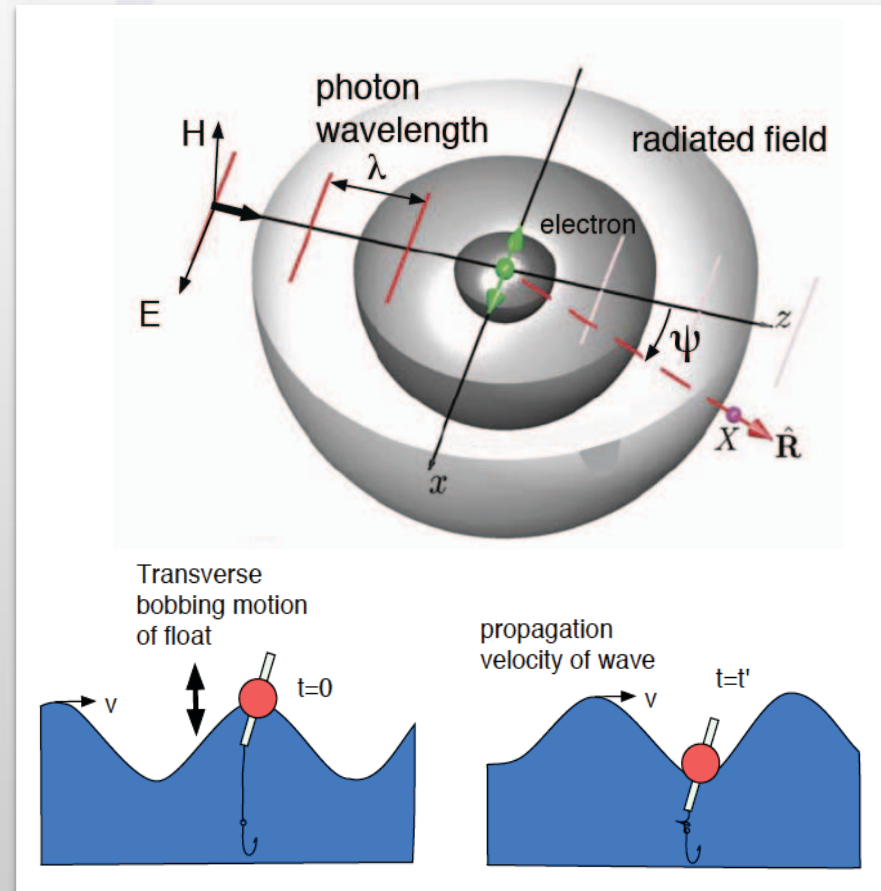
Radiated spherical field  $E_{rad}$  :

- proportional to the electron acceleration
- anti-phase with respect  $E_{in}$
- decreases with  $\cos(\psi)$

$$\frac{E_{rad}(R, t)}{E_{in}} = - \left( \frac{e^2}{4\pi\epsilon_0 mc^2} \right) \frac{e^{ikR}}{R} \cos \psi$$

Thomson scattering length:

$$r_0 = \left( \frac{e^2}{4\pi\epsilon_0 mc^2} \right) = 2.82 \times 10^{-5} \text{ \AA}$$

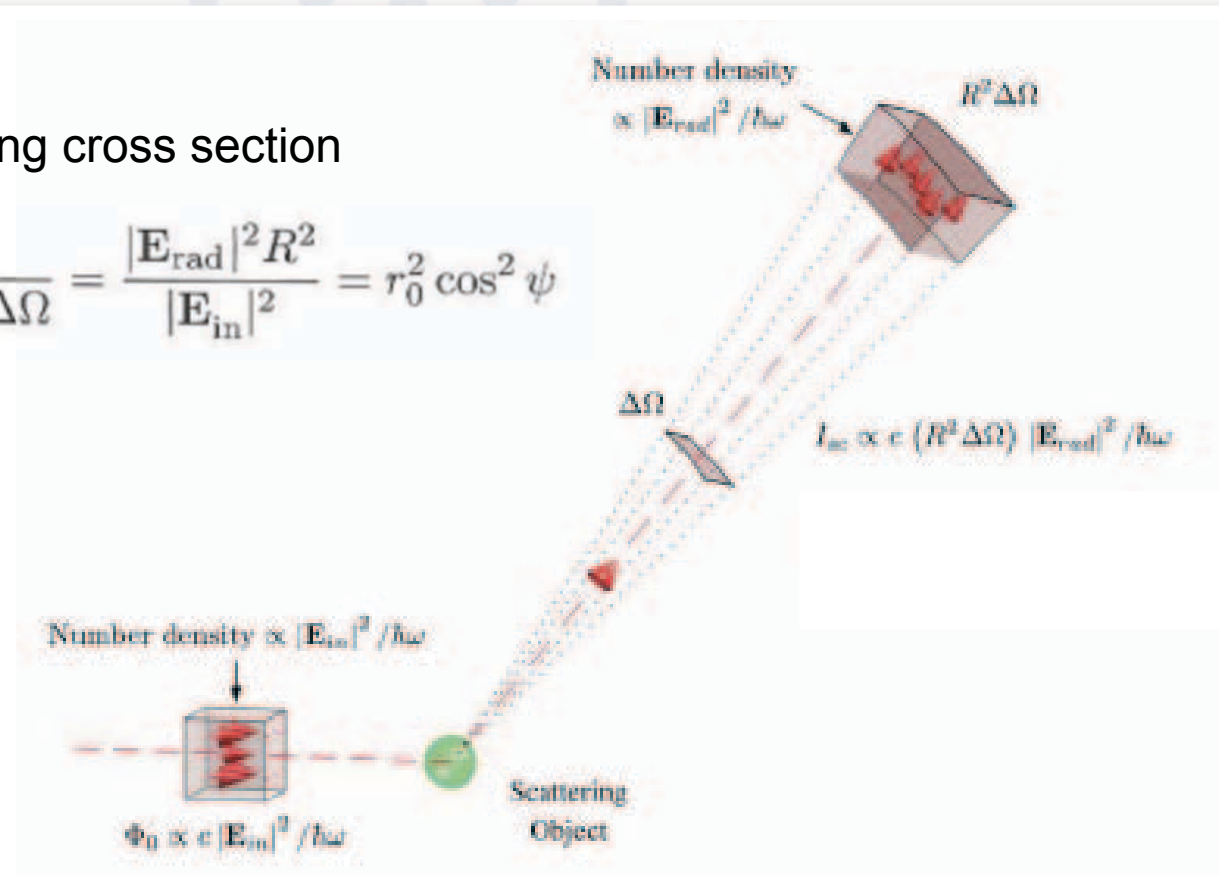


Def.: Thomson differential cross section

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{\text{(Number of X-rays scattered per second into } \Delta\Omega\text{)}}{\text{(Incident flux)}(\Delta\Omega)}$$

Thomson scattering cross section

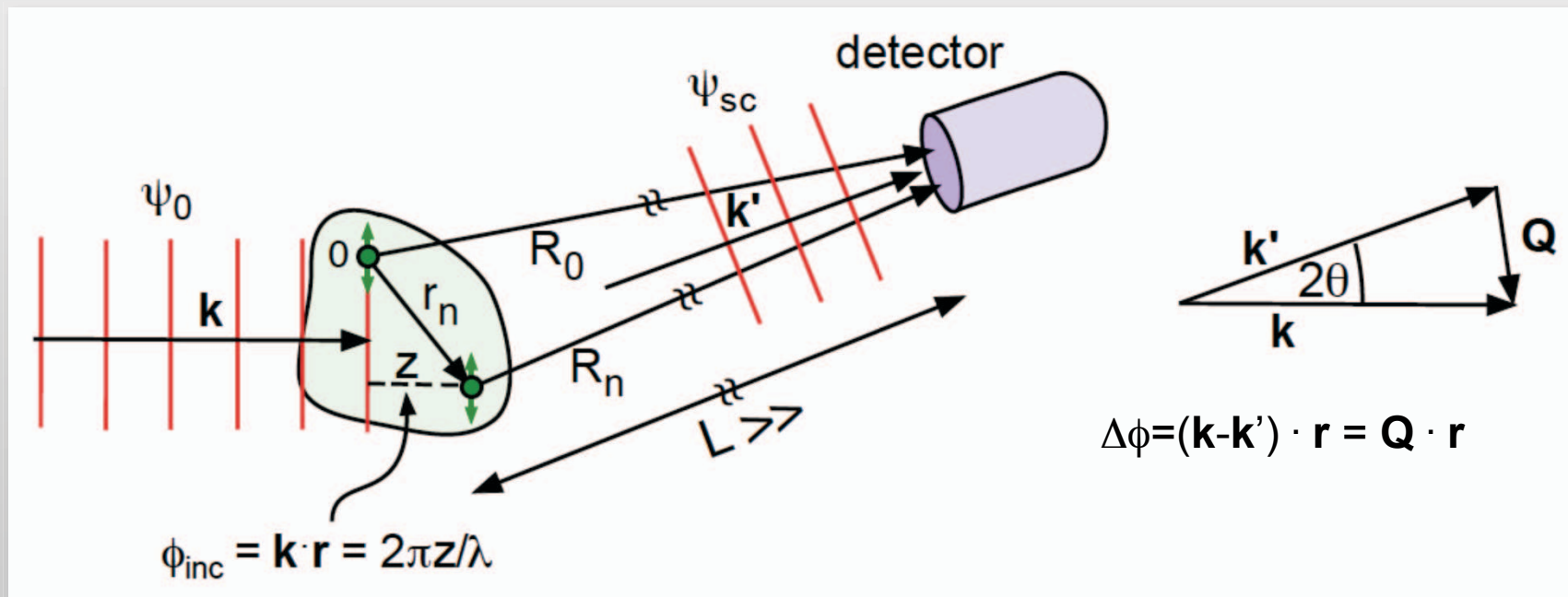
$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{I_{sc}}{(I_0/A_0)\Delta\Omega} = \frac{|\mathbf{E}_{rad}|^2 R^2}{|\mathbf{E}_{in}|^2} = r_0^2 \cos^2 \psi$$



- Interference between scattered X-rays observed in the direction  $\mathbf{k}'$  and at large distances (far field limit), with  $|\mathbf{k}| = |\mathbf{k}'| = 2\pi/\lambda$ .
- The incident wave  $\mathbf{k}$  arrives at the second electron at  $\mathbf{r}_n$  with a phase shift  $\phi_{\text{inc}}$
- The phase difference between the two scattered X-rays is  $\Delta\phi = (\mathbf{k} - \mathbf{k}') \cdot \mathbf{r} = \mathbf{Q} \cdot \mathbf{r}$

$$\frac{d\sigma}{d\Omega} = \frac{|\psi_{\text{sc}}|^2}{|\psi_0|^2} L^2 = 2r_0^2 [1 + \cos(\mathbf{Q} \cdot \mathbf{r}_n)]$$

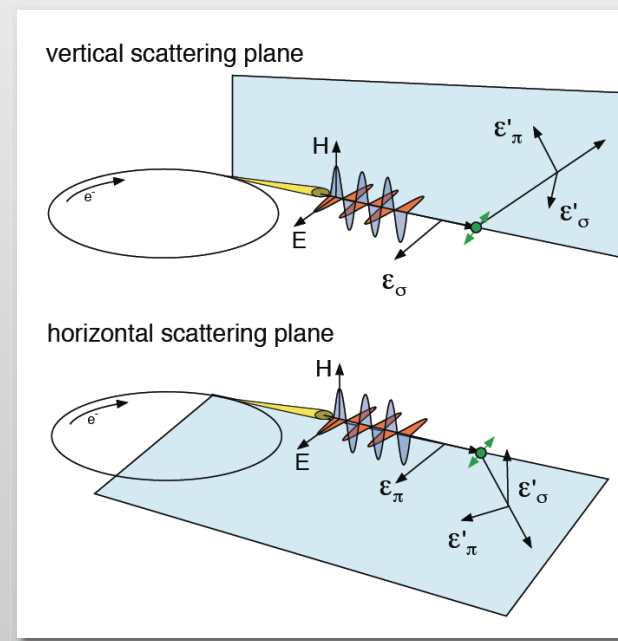
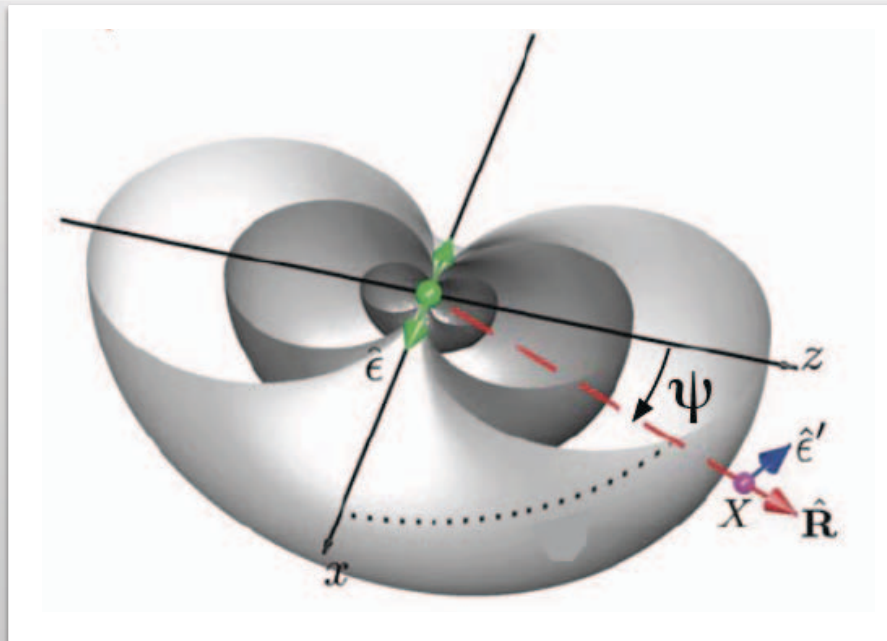
Elastic scattering cross section





The differential cross section for the Thomson scattering depends from the incident and scattered photon polarizations

$$\left(\frac{d\sigma}{d\Omega}\right) = r_0^2 |\hat{\epsilon} \cdot \hat{\epsilon}'|^2 \quad P = |\hat{\epsilon} \cdot \hat{\epsilon}'|^2 = \begin{cases} 1 & \text{synchrotron: vertical scattering plane} \\ \cos^2 \psi & \text{synchrotron: horizontal scattering plane} \\ \frac{1}{2}(1 + \cos^2 \psi) & \text{unpolarized source} \end{cases}$$



The scattering intensity depends from the relative orientation of scattering vector  $Q$  and the vector  $r_n$ .

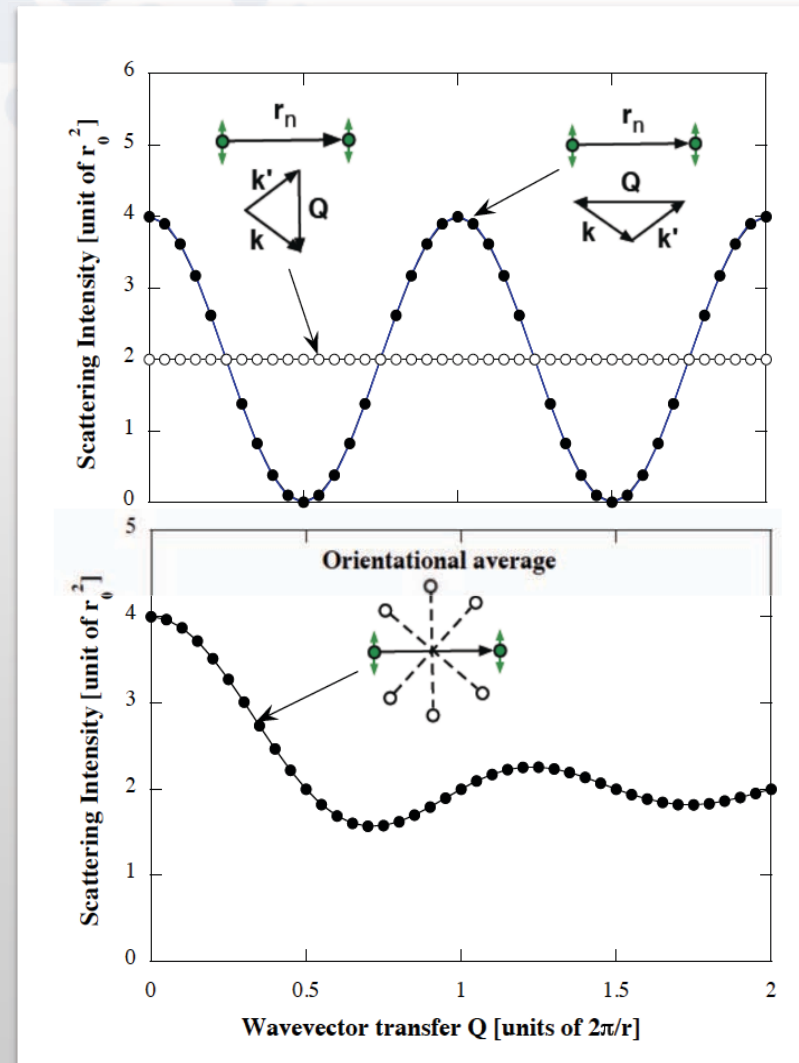
Scattering intensity (two electrons)

$$\frac{d\sigma}{d\Omega} = 2r_0^2(1 + \cos(\mathbf{Q} \cdot \mathbf{r}))$$

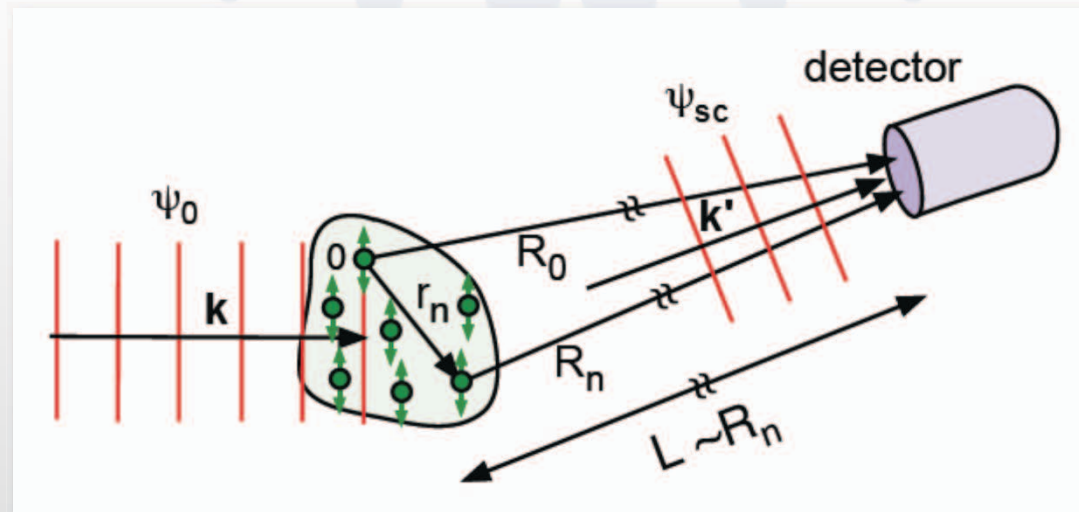
Scattering intensity (two electrons):  
orientational average

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle_{\text{or.av.}} = 2r_0^2(1 + \langle e^{i\mathbf{Q} \cdot \mathbf{r}} \rangle_{\text{or.av.}})$$

$$\langle e^{i\mathbf{Q} \cdot \mathbf{r}} \rangle_{\text{or.av.}} = \frac{\sin(Qr)}{Qr}$$



In general if we have a random distribution of electrons, the scattering function is obtained sum coherently all the individual terms



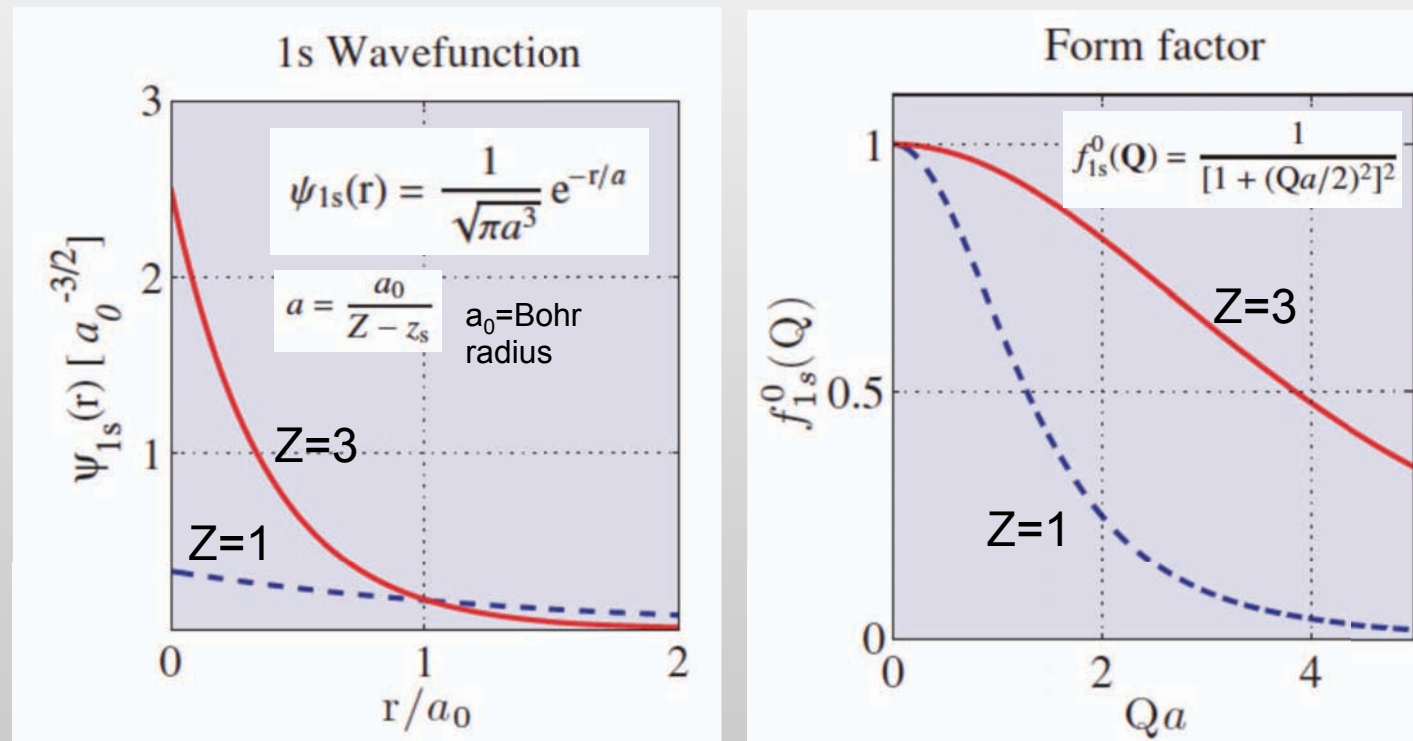
$$\begin{aligned}
 \psi^{sc} &= \sum_n \psi_n^{sc} = \sum_n -r_0 \frac{e^{ik \cdot \mathbf{R}_n}}{R_n} \\
 &\approx \frac{1}{L} \sum_n -r_0 e^{ik \cdot \mathbf{R}_n} = \frac{1}{L} \sum_n -r_0 e^{ik \cdot (\mathbf{R}_0 + \mathbf{r}_n)} \\
 &= \frac{1}{L} \sum_n -r_0 e^{ik \cdot \mathbf{r}_n}
 \end{aligned}$$

$$\frac{d\sigma}{d\Omega} = r_0^2 \left| \sum_n e^{i\mathbf{Q} \cdot \mathbf{r}_n} \right|^2$$

The form factor is related to the Fourier transform of charge density distribution:

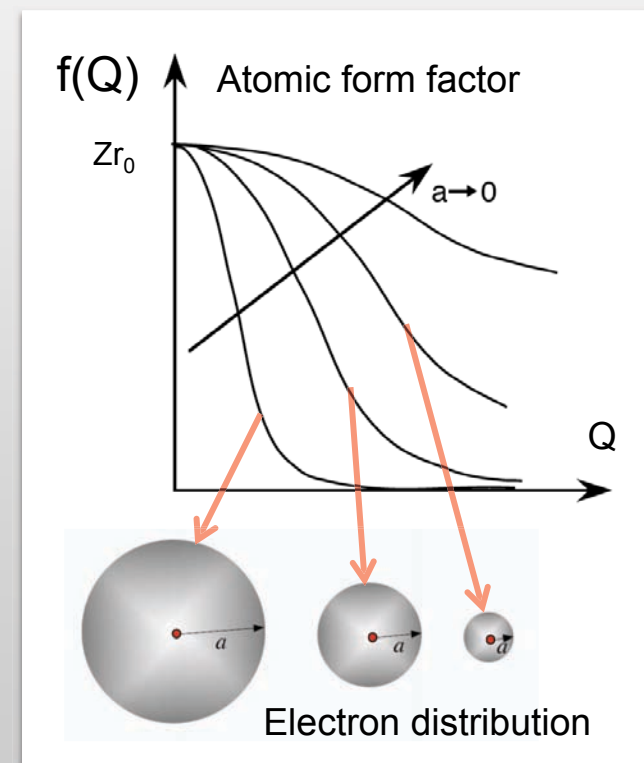
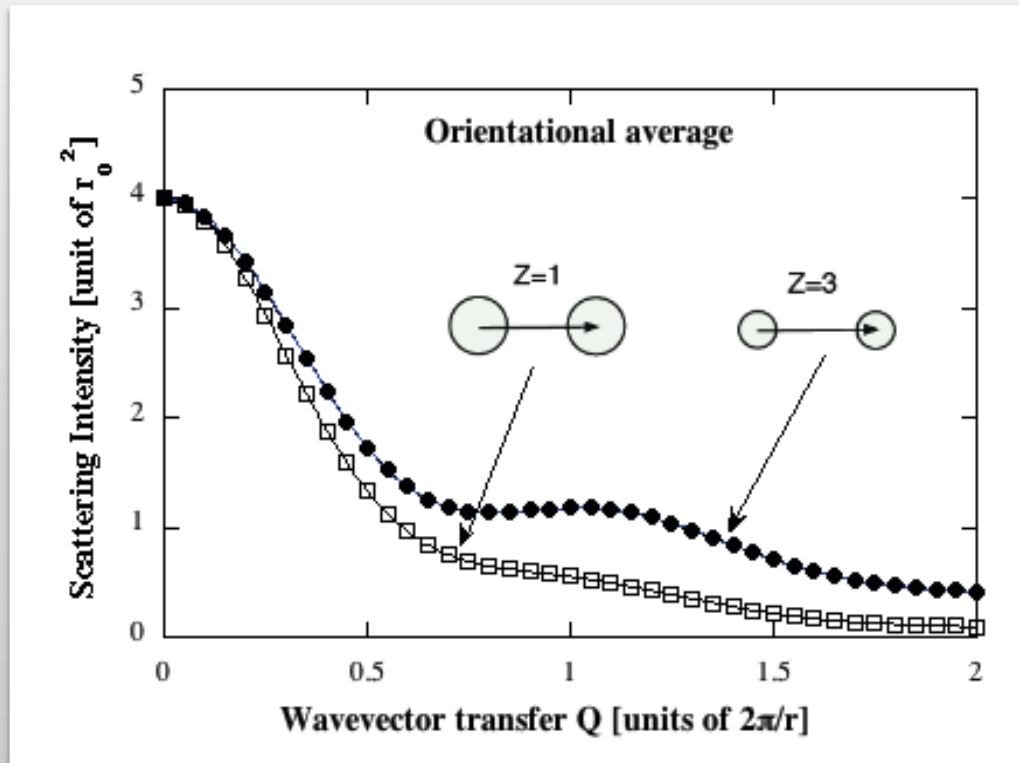
$$f^0(\mathbf{Q}) = -r_0 \int \rho(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} d\mathbf{r} = \begin{cases} Z & \text{for } \mathbf{Q} \rightarrow 0 \\ 0 & \text{for } \mathbf{Q} \rightarrow \infty \end{cases}$$

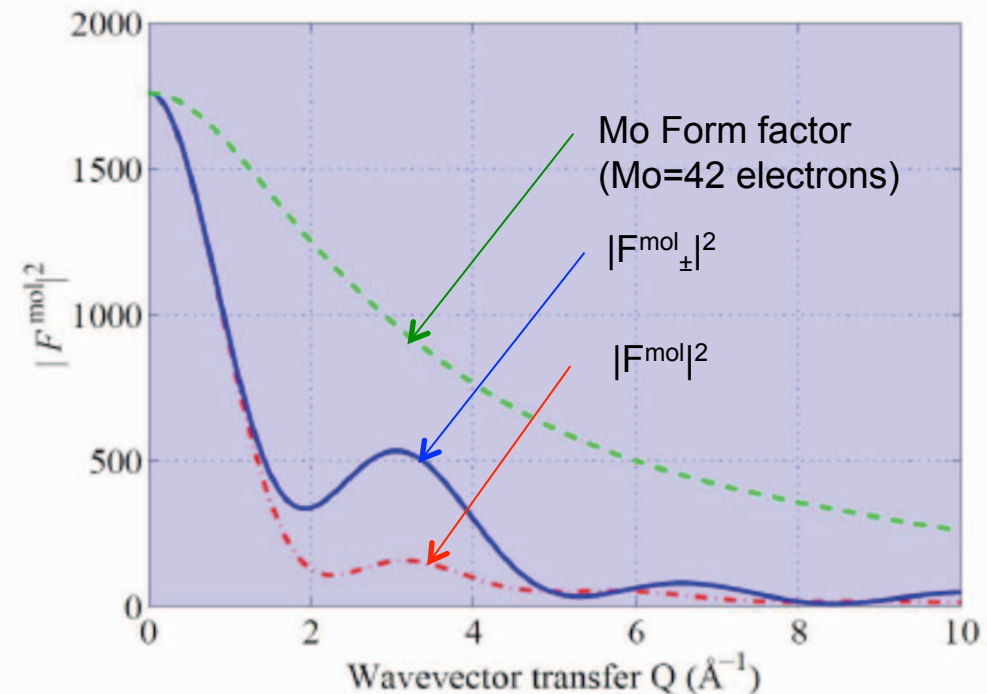
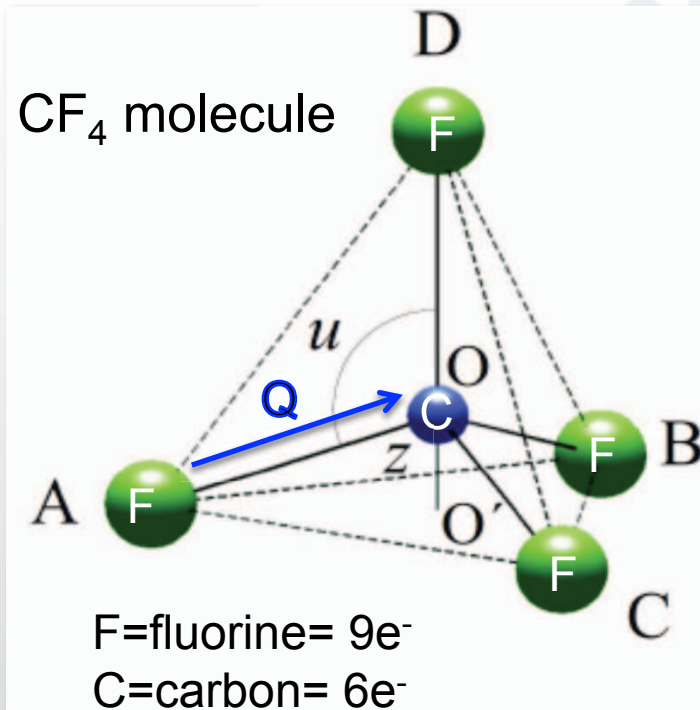
The Q dependence is due to the fact that the Thomson scattering is produced by all atomic electrons, which have a spatial extent of the same order of magnitude as the X-ray wavelength.



The scattering of two atoms which have a spatial extent of electron distribution of the same order of magnitude as the X-ray wavelength.

$$\langle I(Q) \rangle_{\text{orient. av.}} = f_1^2 + f_2^2 + 2 f_1 f_2 \langle e^{iQ \cdot r} \rangle_{\text{orient. av.}}$$





Molecular structure factors 
$$F^{\text{mol}}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$

$Q \parallel$  C-F bond

$$F^{\text{mol}}_{\pm}(\mathbf{Q}) = f^{\text{C}}(\mathbf{Q}) + f^{\text{F}}(\mathbf{Q}) \left[ 3e^{\mp iQR/3} + e^{\pm iQR} \right]$$

Orientational average

$$|F^{\text{mol}}|^2 = |f^{\text{C}}|^2 + 4|f^{\text{F}}|^2 + 8f^{\text{C}}f^{\text{F}} \frac{\sin(QR)}{QR} + 12|f^{\text{F}}|^2 \frac{\sin(Q\sqrt{8/3}R)}{Q\sqrt{8/3}R}$$

Cristalline solids exhibit long range structural order and sit on a regular array. Amorphous materials present a degree of randomness in the position of the atoms and the structural order, if present at all, can only be described in a statistical sense.

Radial density

$$2D \quad N(r)/2\pi r dr$$

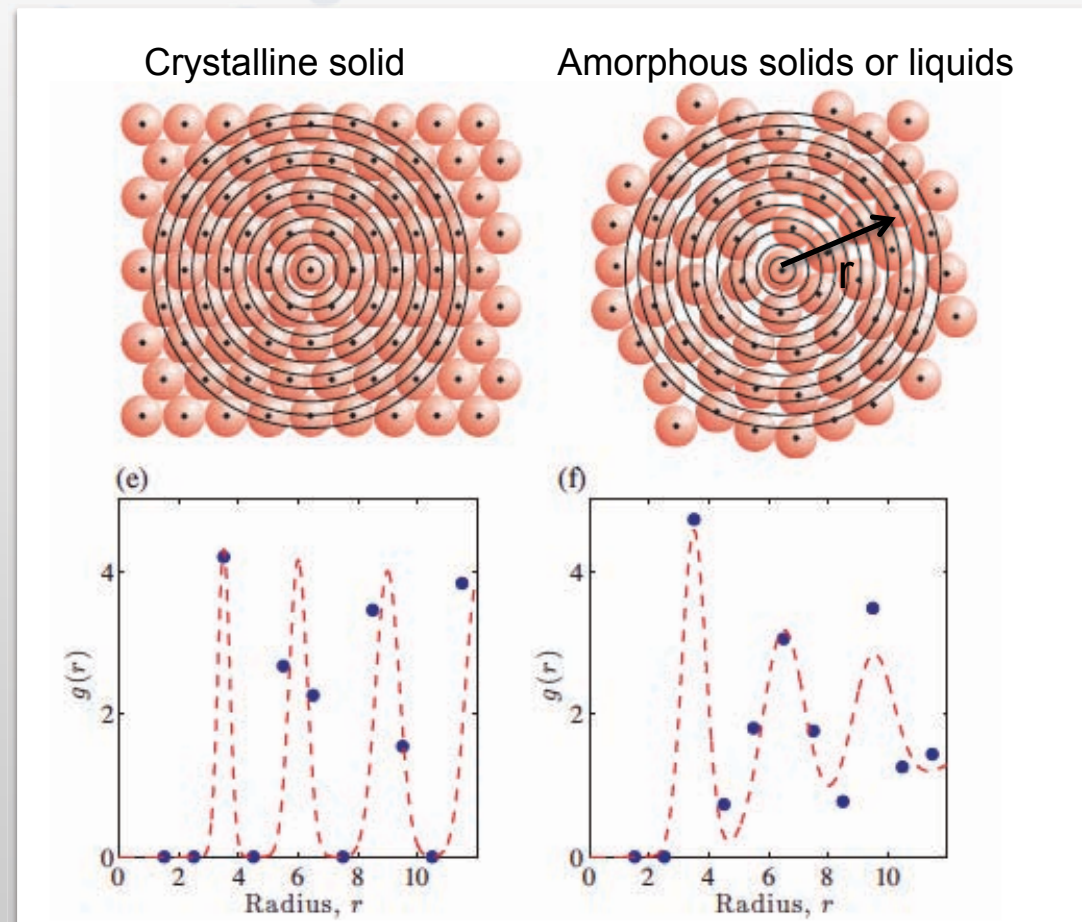
$$3D \quad N(r)/4\pi r^2 dr$$

Radial distribution function

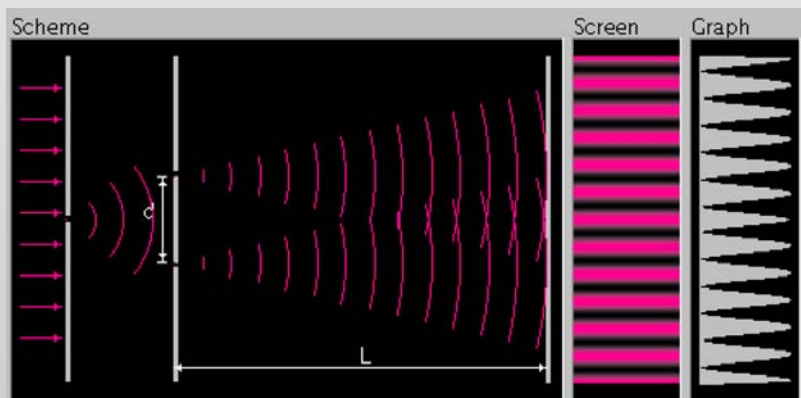
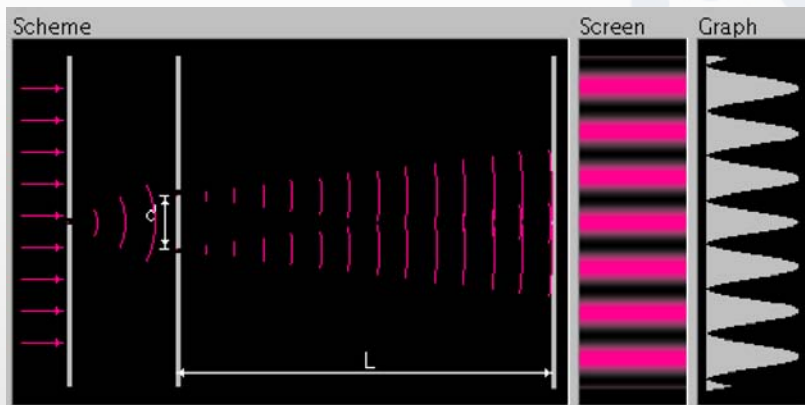
$$g(r) = \rho(r) / \rho_{at}$$

$$g(r) \rightarrow 1 \quad \rho(r) \rightarrow \rho_{at}$$

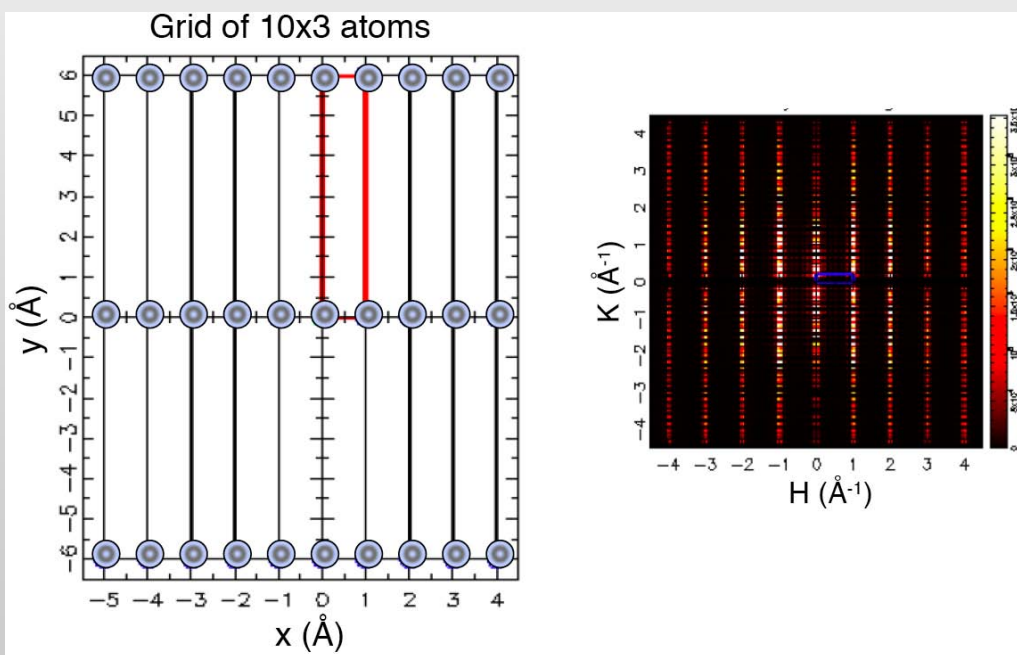
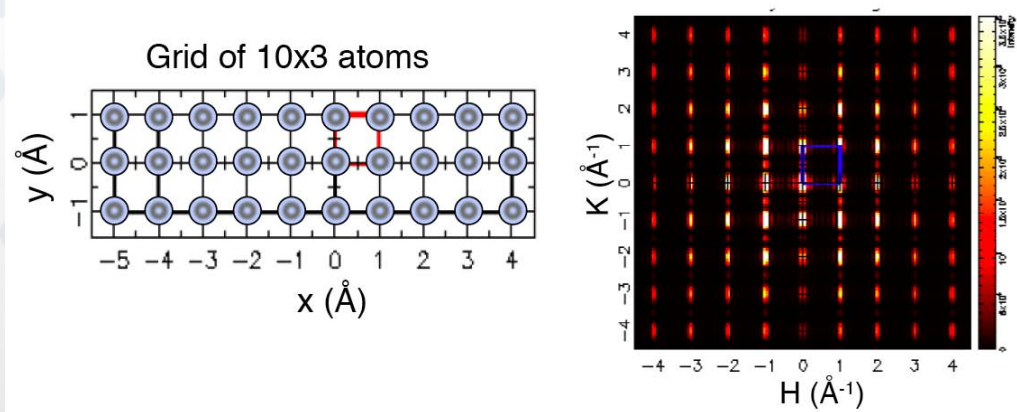
The radial distribution function can be obtained from the Fourier transform of the observed intensity as a function of wavevector transform  $Q$ .



## Visible light interference

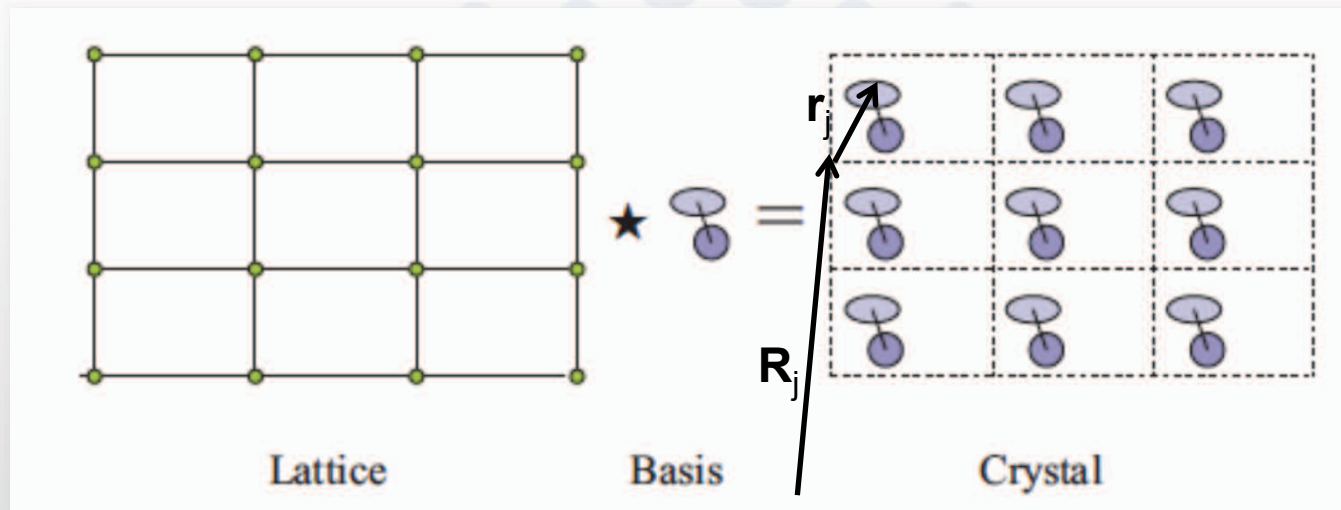


## X-rays diffraction by atoms



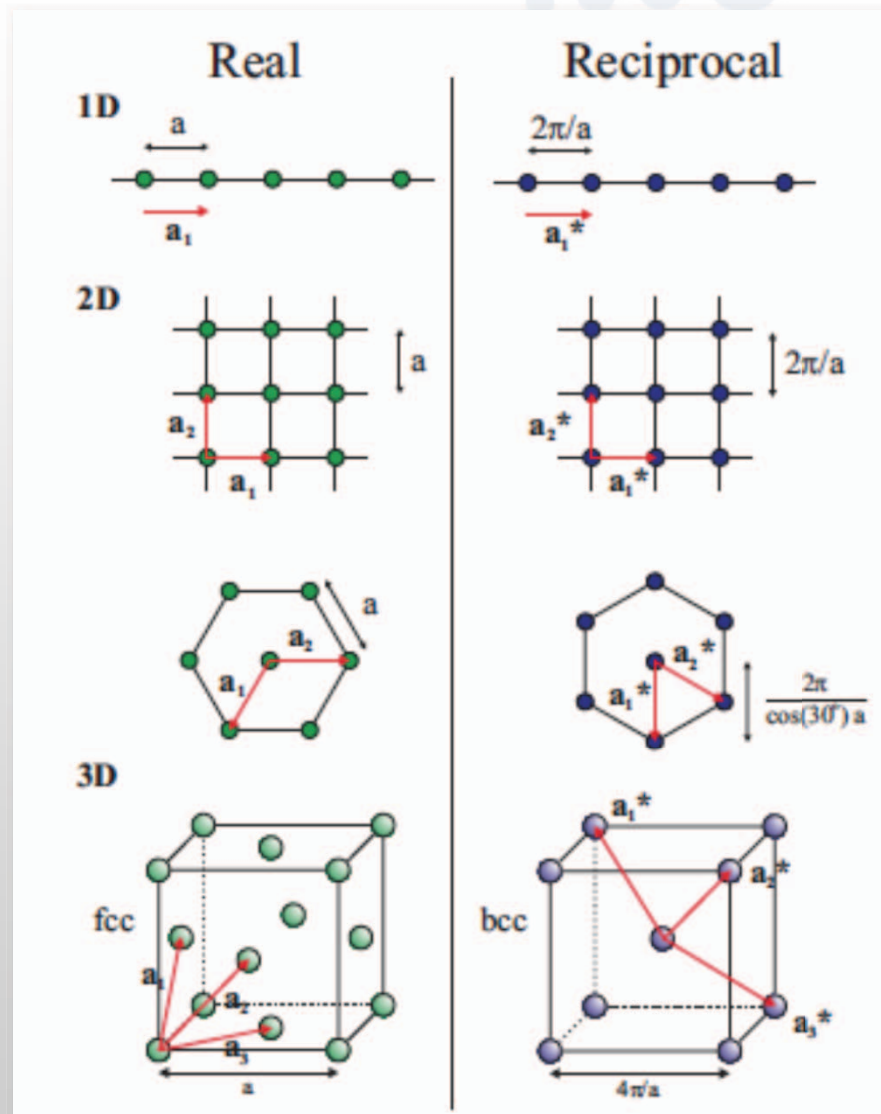


A two-dimensional crystal structure is built from the convolution of a lattice and a basis.



The Structure factor could be written as a product between the lattice sum and the unit cell structure factor.

$$F^{crystal}(\mathbf{Q}) = \sum_{\mathbf{R}_n + \mathbf{r}_j}^{\text{All atoms}} f_j(\mathbf{Q}) e^{i\mathbf{Q} \cdot (\mathbf{R}_n + \mathbf{r}_j)} = \underbrace{\sum_n e^{i\mathbf{Q} \cdot \mathbf{R}_n}}_{\text{Lattice}} \underbrace{\sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q} \cdot \mathbf{r}_j}}_{\text{Unit cell}}$$



Maximization of the lattice sum

$$\sum_n e^{i\mathbf{Q}\cdot\mathbf{R}_n} \quad \mathbf{Q}\cdot\mathbf{R}_n = 2\pi \times \text{integer}$$

Definition of reciprocal space

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi \delta_{ij} \quad \mathbf{G} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$$

$$\mathbf{a}_1^* = \frac{2\pi}{V_c} \mathbf{a}_2 \times \mathbf{a}_3 \quad \mathbf{a}_2^* = \frac{2\pi}{V_c} \mathbf{a}_3 \times \mathbf{a}_1 \quad \mathbf{a}_3^* = \frac{2\pi}{V_c} \mathbf{a}_1 \times \mathbf{a}_2$$

Laue condition for x-ray diffraction

$$\mathbf{Q} = \mathbf{G}$$

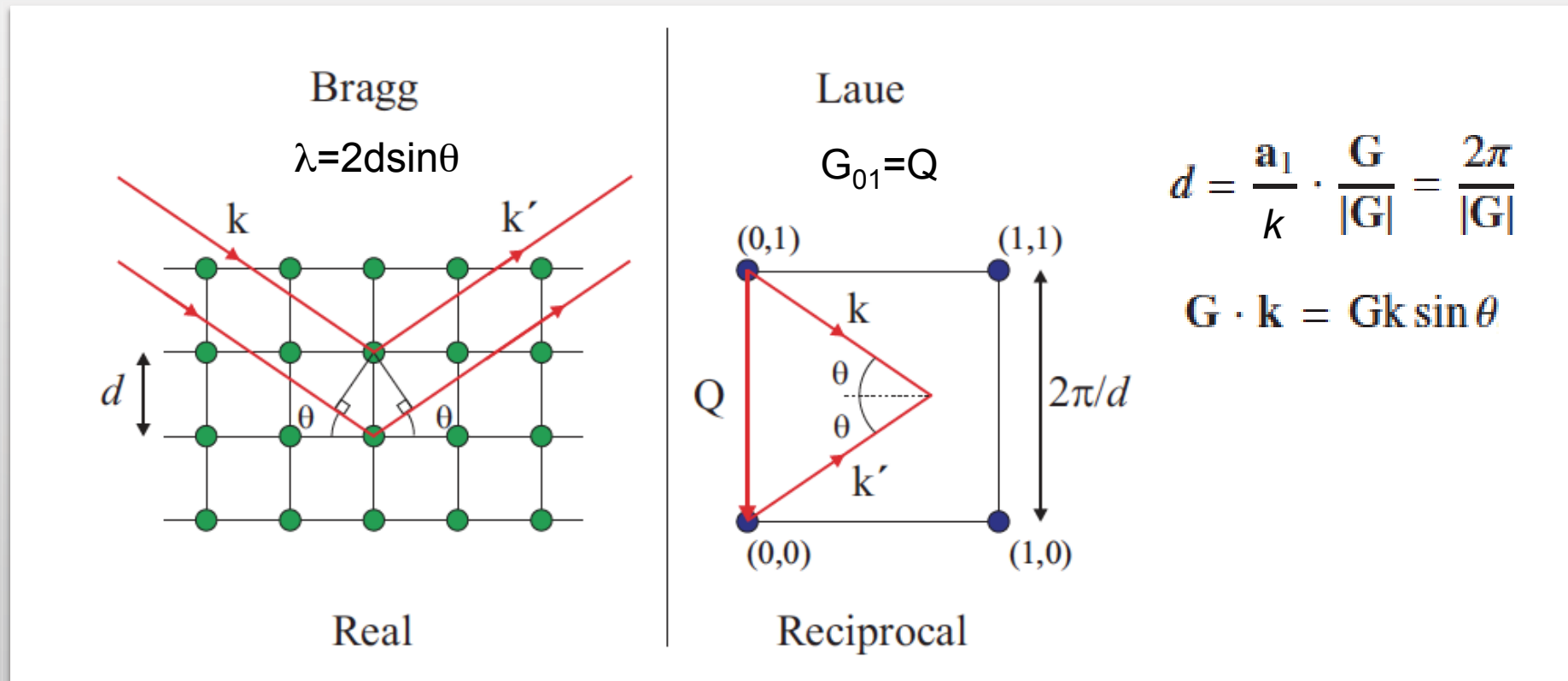
$$\mathbf{G} \cdot \mathbf{R}_n = 2\pi(hn_1 + kn_2 + ln_3)$$

Bragg condition for x-ray elastic diffraction:

the path length difference between the incident  $k$  and reflected  $k'$  waves is an integer multiple of their wavelength  $\lambda$ .

The Bragg and Laue conditions are equivalent:

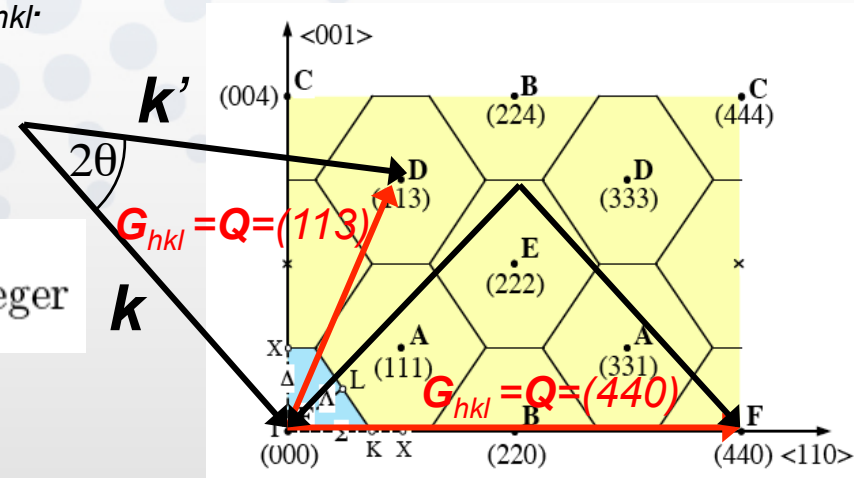
- $G_{hkl}$  is perpendicular to the planes with Miller indices  $(hkl)$ .
- $|G_{hkl}|$  is equal to the inverse of lattice spacing  $d_{hkl}$  of  $(hkl)$  planes



**- The Laue's condition**

the scattering intensities are non-vanishing when the scattering vector  $Q=k-k'$  coincides with a reciprocal lattice vector  $G_{hkl}$ :

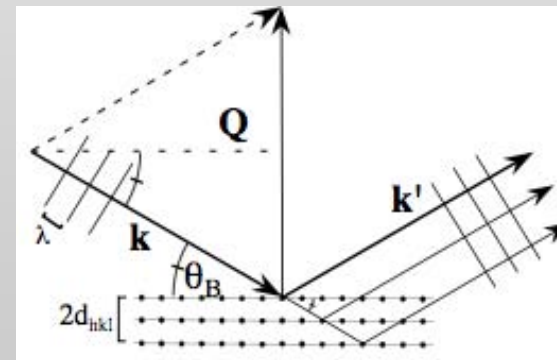
$$Q \cdot R_n = 2\pi (hn_1 + kn_2 + ln_3) = 2\pi \cdot \text{integer}$$



**-The Bragg's law**

interference condition between an incident and a reflected waves by a periodic arrangement of atoms.

$$n \lambda = 2 d_{hkl} \sin\theta_B$$



- The Structure factor  $F(hkl)$  describes the interference between the resultant waves diffused from each atom in the unit cell for any given reciprocal lattice vector  $\mathbf{Q} = \mathbf{G}_{hkl}$  i.e.:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{Bragg}} = N \frac{(2\pi)^3}{v_0} \sum_{hkl} \delta(\mathbf{Q} - \mathbf{G}_{hkl}) |F(hkl)|^2$$

$N^\circ$  unit cell

unit cell volume

Laue's condition

$$F(hkl) = \sum_s f_s e^{i\mathbf{G}_{hkl} \cdot \mathbf{d}_s - W_s}$$

Structure factor: information about the atom distribution inside the unit cell

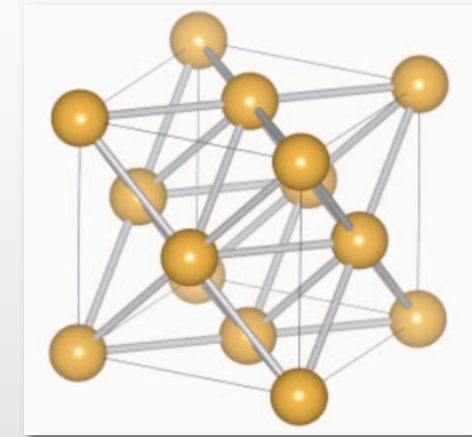
$$f_s = \int_{\text{atom}} \rho_s(\mathbf{r}') e^{-i\mathbf{Q} \cdot \mathbf{r}'} d\mathbf{r}'$$

$f_s$  = atomic scattering amplitude for the atoms  $s$  related to the Fourier transform of the atomic electron density

Example: FCC lattice

Composed by four atoms at  $(000)$ ,  $(\frac{1}{2}\frac{1}{2}0)$ ,  $(0\frac{1}{2}\frac{1}{2})$  and  $(\frac{1}{2}0\frac{1}{2})$  unit cell positions

$$\begin{aligned}
 F_{hkl}^{fcc} &= f(\mathbf{G}) \sum_j e^{i\mathbf{G}\cdot\mathbf{r}_j} \\
 &= f(\mathbf{G})(1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(l+h)}) \\
 &= f(\mathbf{G}) \times \begin{cases} 4 & \text{if } h, k, l \text{ are all even or all odd} \\ 0 & \text{otherwise} \end{cases}
 \end{aligned}$$

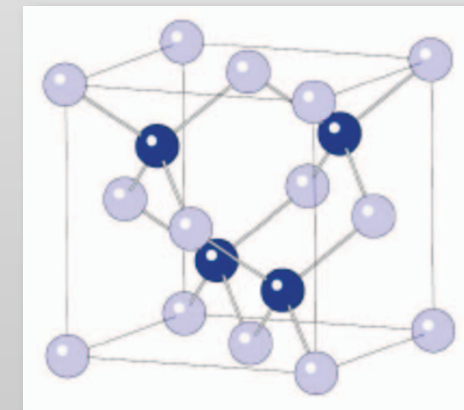


Example: AsGa (Zinc-blende)

convolution of a FCC lattice and a “motif” of two atoms at  $(000)$  and  $(\frac{1}{4}\frac{1}{4}\frac{1}{4})$

$$\begin{aligned}
 F_{hkl}^{\text{GaAs}} &= (1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(l+h)}) \\
 &\quad \times (f^{\text{Ga}}(\mathbf{G}) + f^{\text{As}}(\mathbf{G})e^{i2\pi(h/4+k/4+l/4)})
 \end{aligned}$$

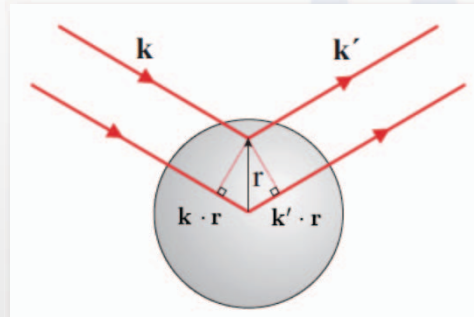
$$F_{200}^{\text{GaAs}} = 4(f^{\text{Ga}}(2, 0, 0) - f^{\text{As}}(2, 0, 0))$$



Scattering processes conserve the number of photons  
 If the photon energy is conserved, the scattering is elastic

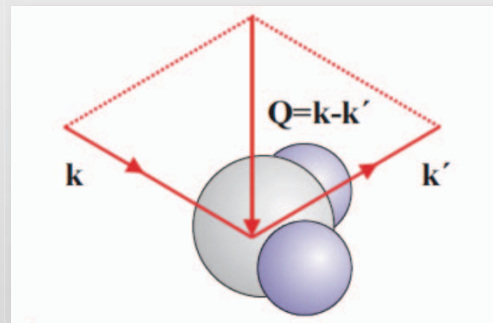
Structure factors

one atom



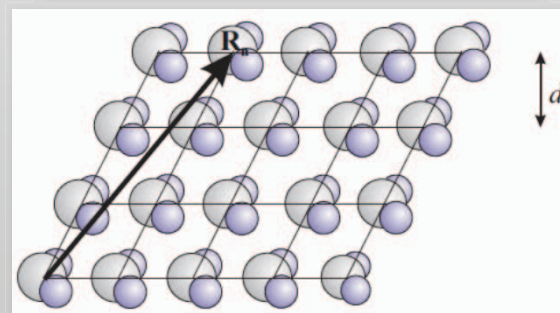
$$-r_0 f^0(\mathbf{Q}) = -r_0 \int \rho(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} d\mathbf{r}$$

a molecule



$$F^{\text{mol}}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q} \cdot \mathbf{r}_j}$$

a crystal



$$F^{\text{crystal}}(\mathbf{Q}) = \underbrace{\sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q} \cdot \mathbf{r}_j}}_{\text{Unit cell structure factor}} \underbrace{\sum_n e^{i\mathbf{Q} \cdot \mathbf{R}_n}}_{\text{Lattice sum}}$$

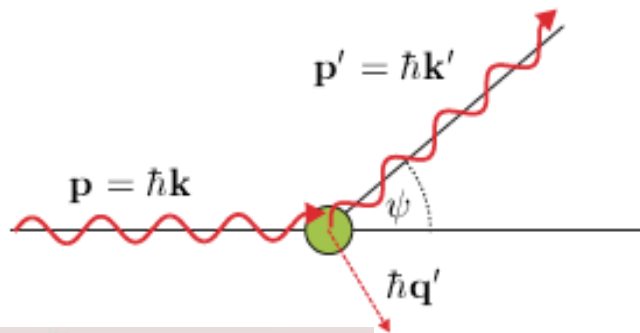
Compton scattering:

Inelastic collision between a photon and an electron at the rest in which the energy is transferred from the photon to the electron.

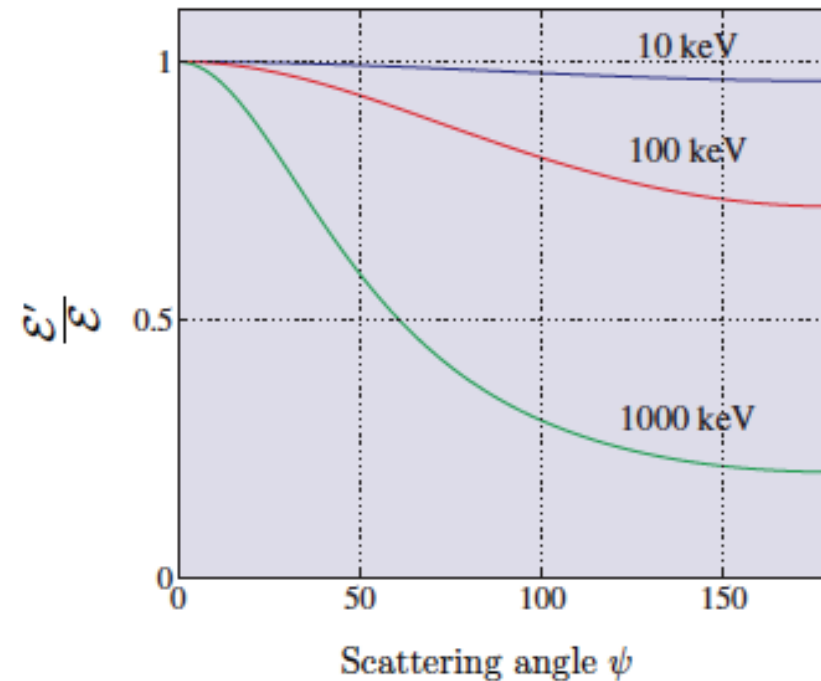
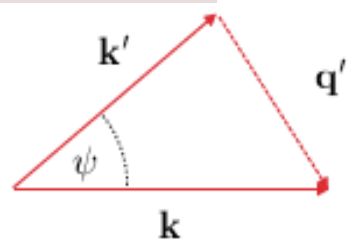
The scattering is **incoherent** because the the photon change its wavelength!

$$\frac{k}{k'} = 1 + \lambda_C k (1 - \cos \psi) = \frac{\mathcal{E}}{\mathcal{E}'} = \frac{\lambda'}{\lambda}$$

$$\lambda_C = \frac{\hbar}{mc} = 3.86 \times 10^{-3} \text{ \AA}$$



$$mc^2 + \hbar ck = \sqrt{(mc^2)^2 + (\hbar cq')^2} + \hbar ck'$$



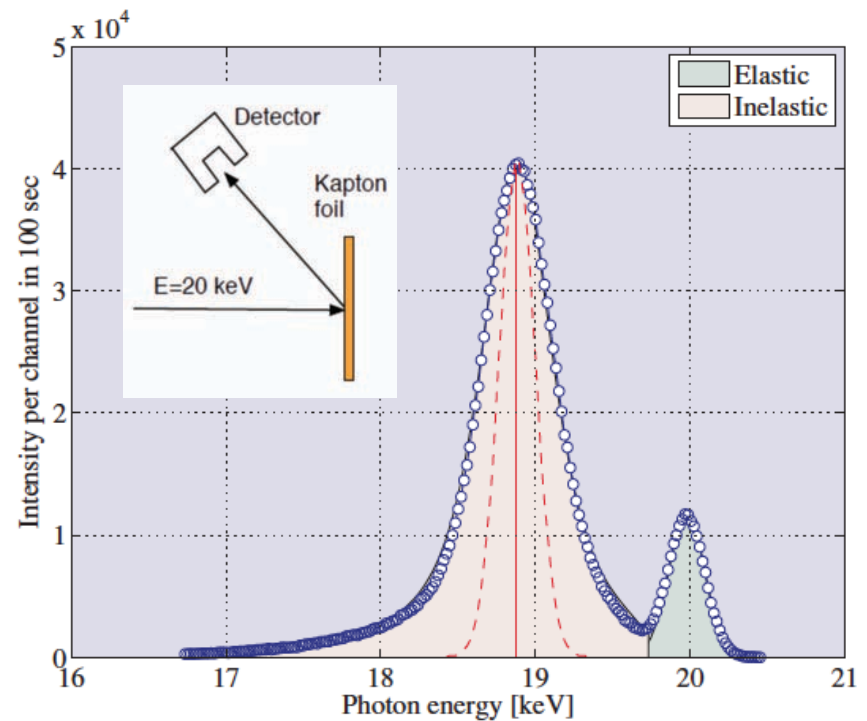
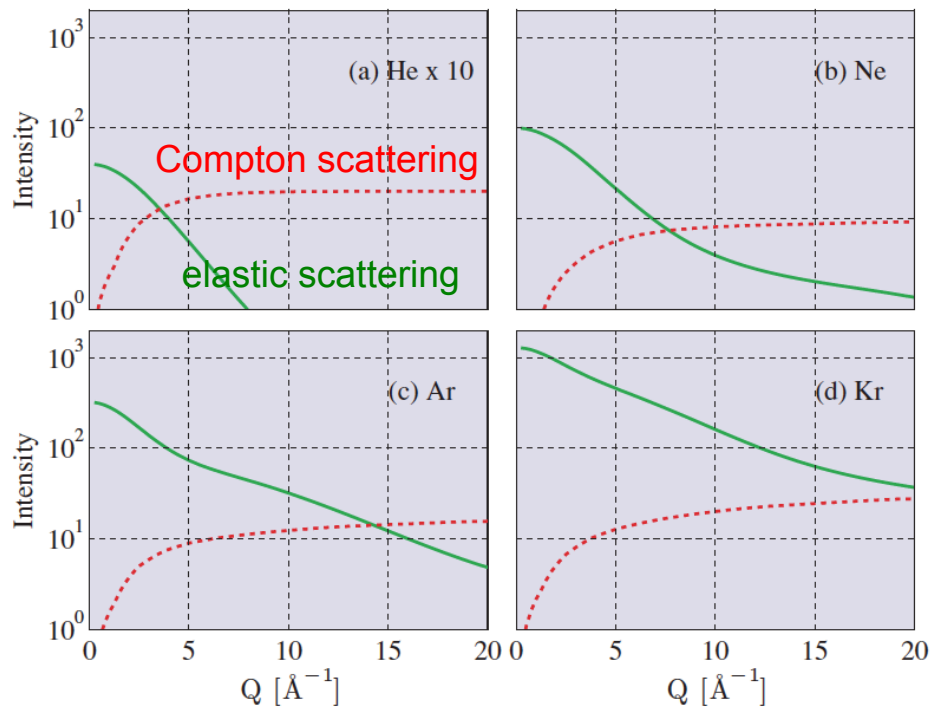


The inelastic scattering dominates at high Q vectors and for low Z elements

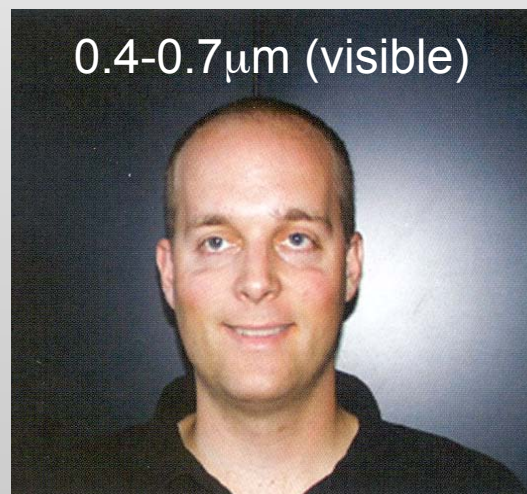
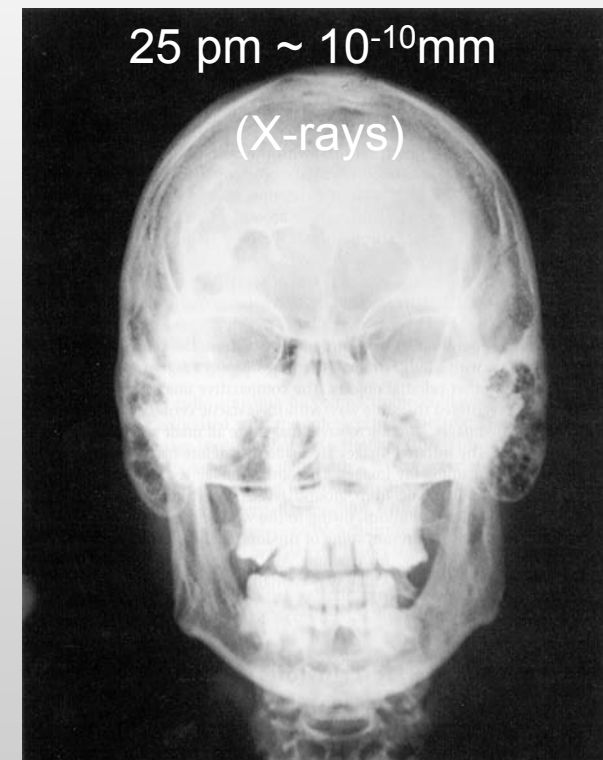
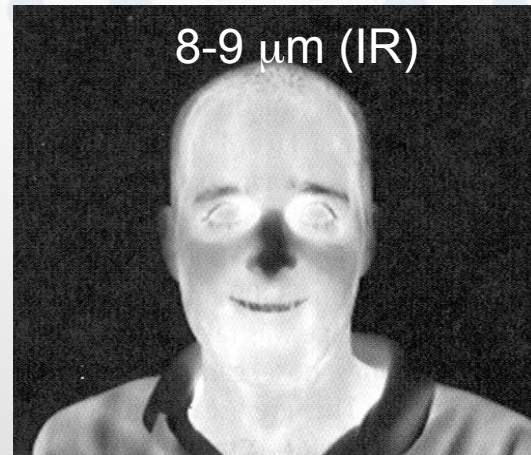
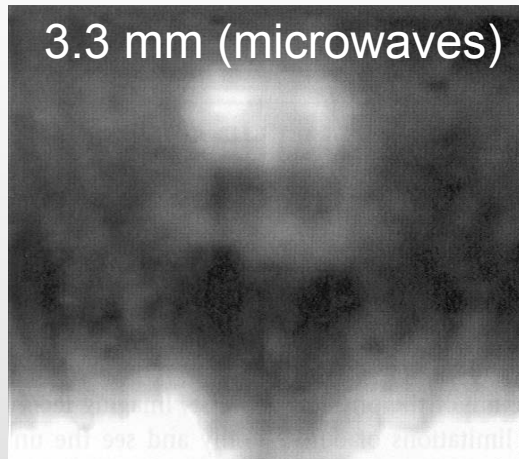
Thomson scattering intensity approach  $Z^2$  when  $Q \rightarrow 0$

Compton scattering approaches  $Z$  when  $Q \rightarrow \infty$

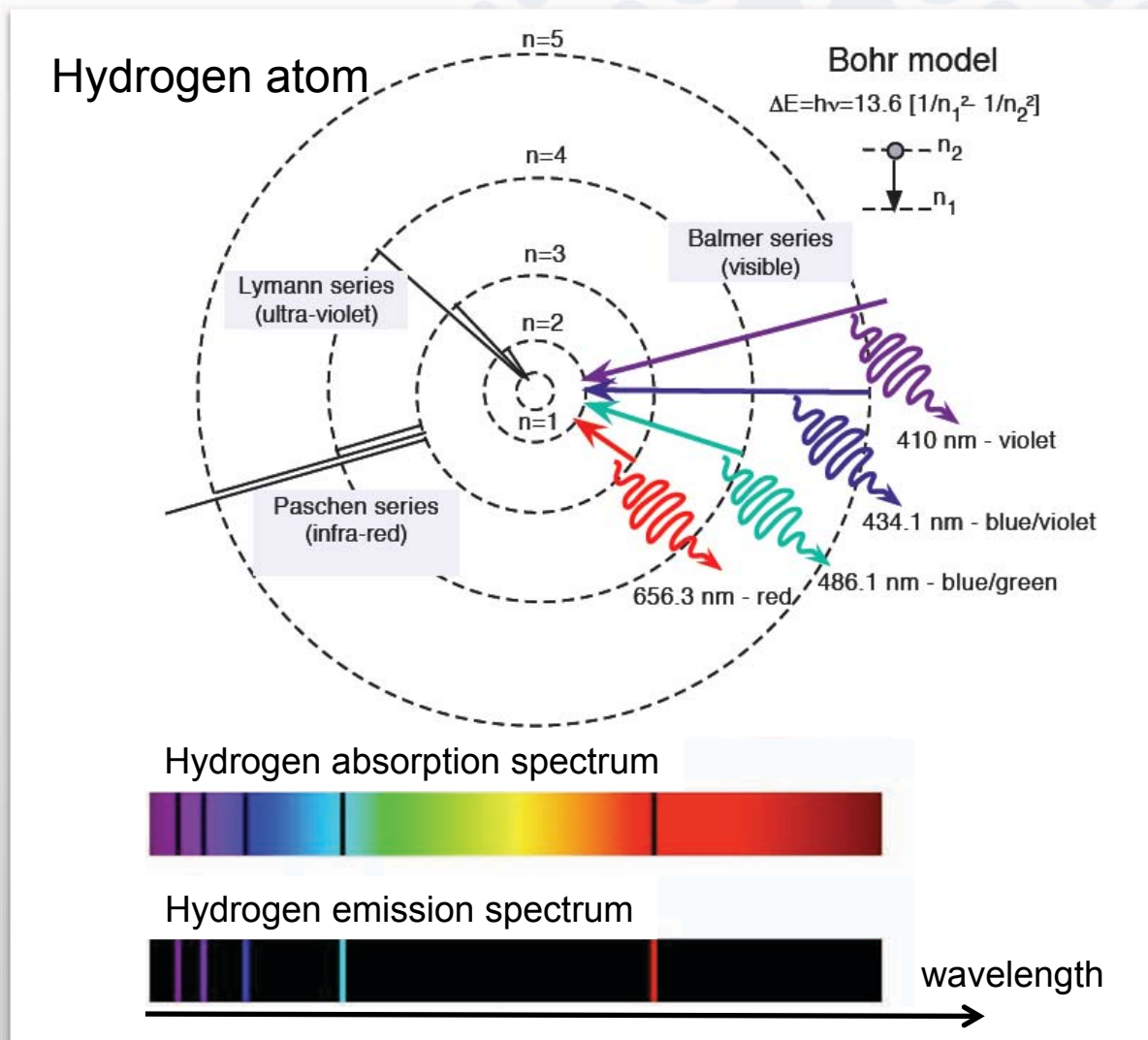
Elastic and inelastic scattering in noble gas



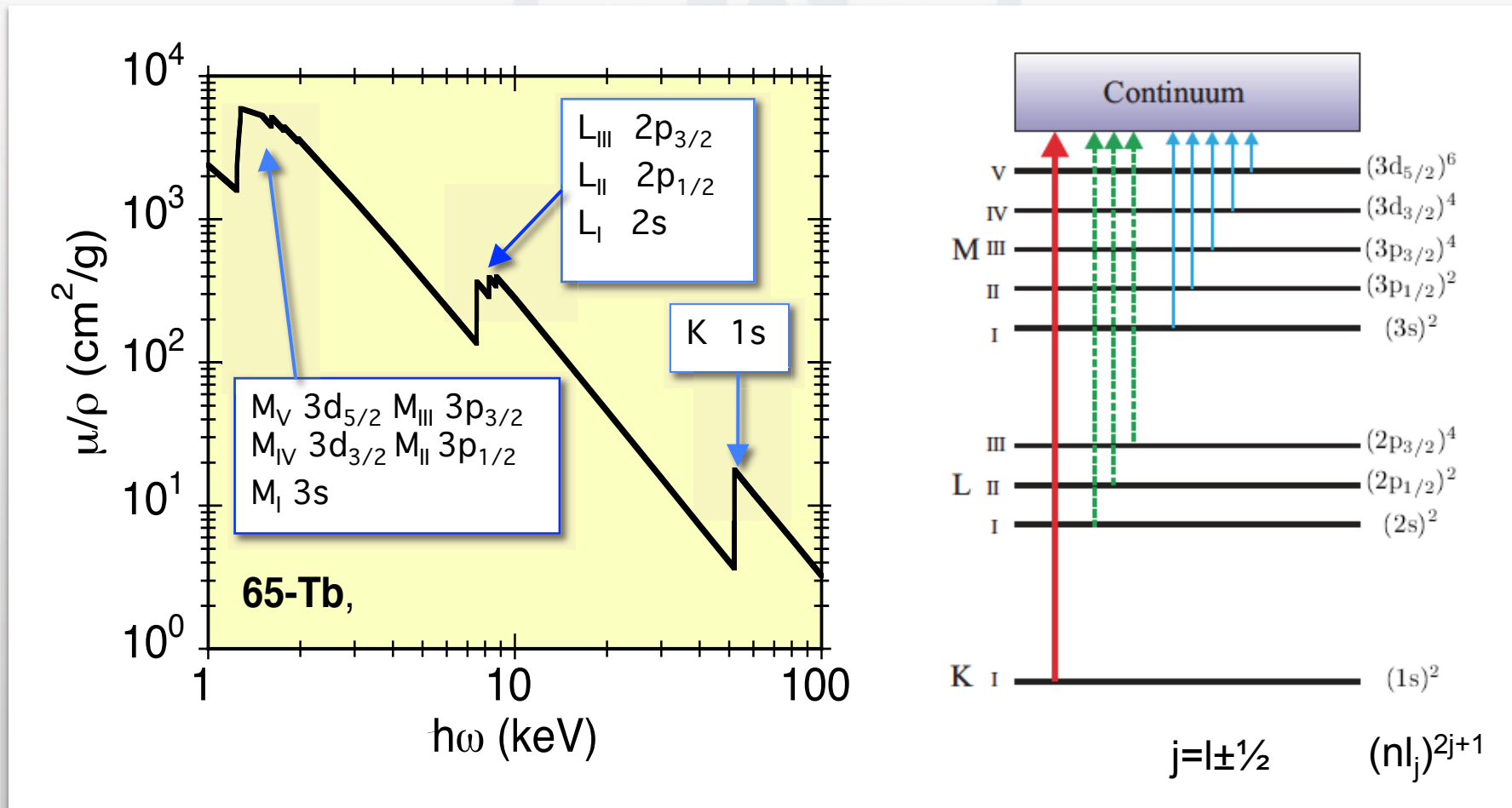
The absorption of electromagnetic radiation change with the wavelength and depends from the characteristic properties of photon/matter interaction.



Photons are adsorbed or re-emitted by atomic electrons at discrete energies.  
 Determination of elemental composition by its electromagnetic response.



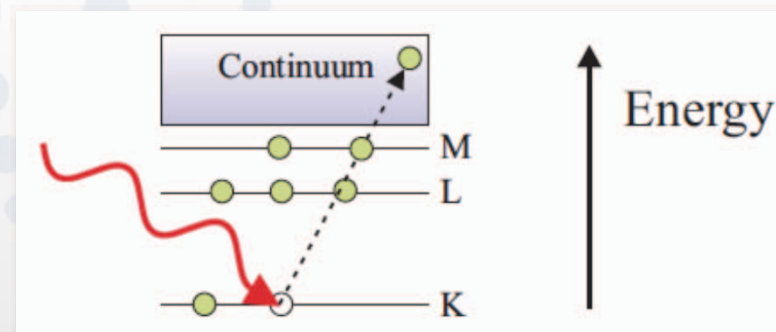
X-rays energies are able to extract atomic electrons from the atomic core!  
 The element-specific energies of the discontinuous jumps in the x-rays absorption spectra are called absorption edges.



Absorption and emission processes are tools for basic analysis of the electronic structure of atom, molecules and solids over different energy scales.

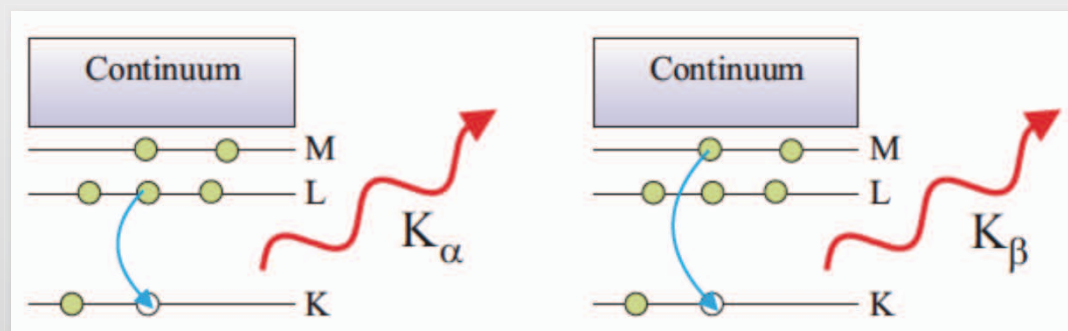
## Photo-electric absorption

Photon absorbed and electron emitted in the continuum



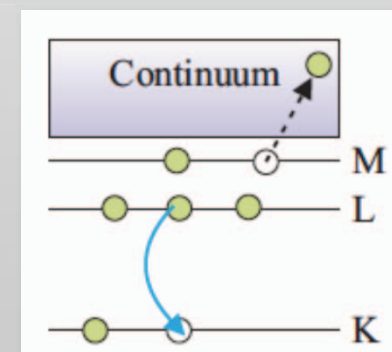
## Fluorescent emission

An electron from the outer shell fills the hole and emits a photon



## Auger electron emission

The atom relaxes into the ground state by emitting an electron

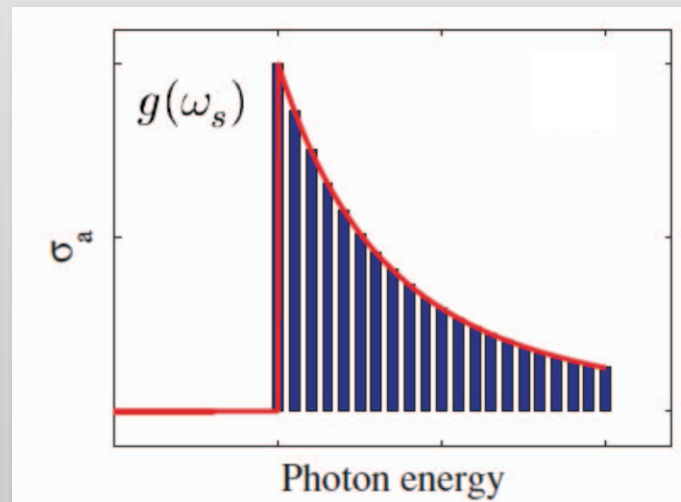


Because the electrons are bound in atoms with discrete energies, a more elaborate model than that of a cloud of free electrons must be invoked.

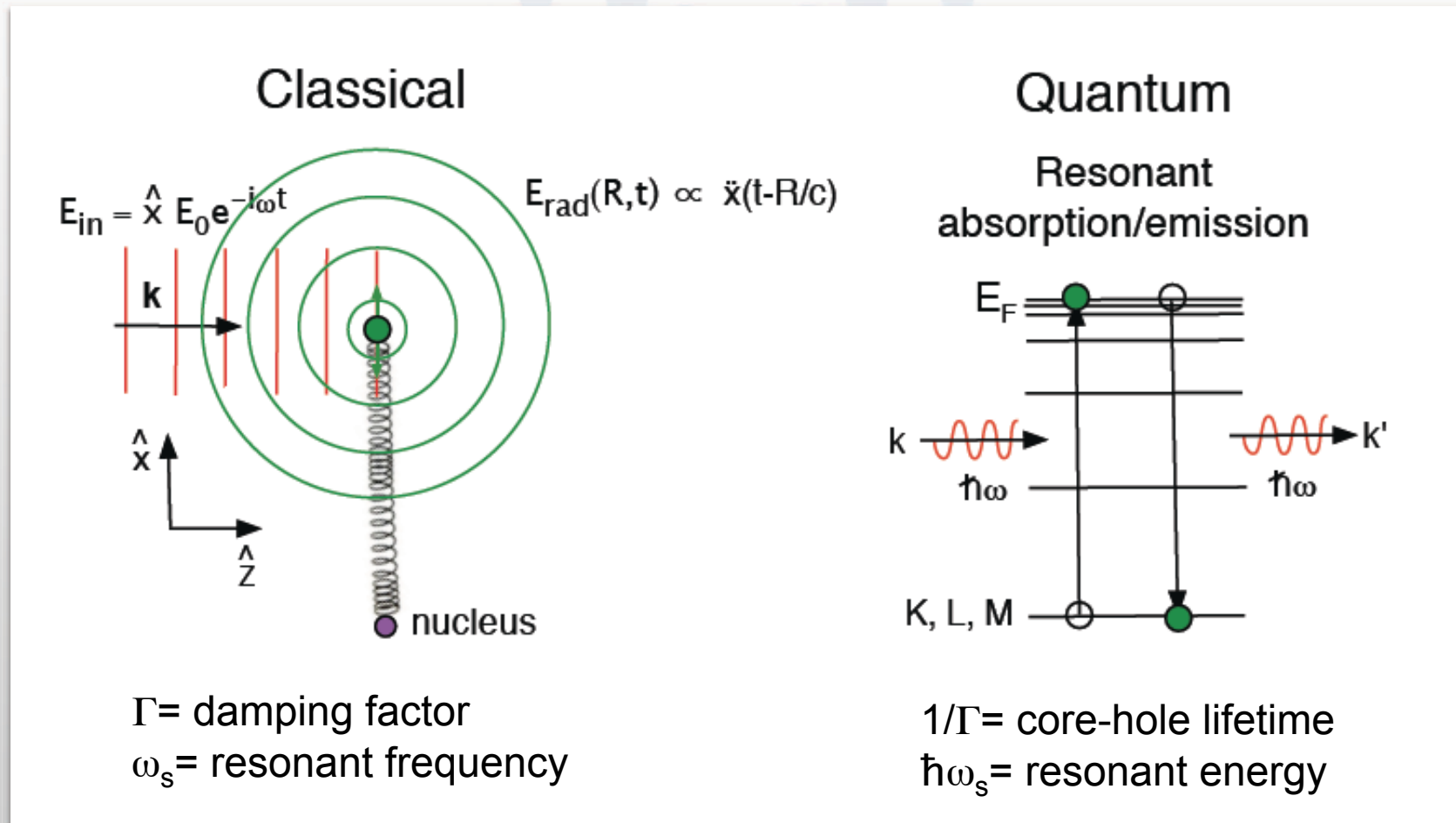
The scattering amplitude includes two energy dependent term  $f'(\omega)$  and  $f''(\omega)$  which are called “dispersion corrections”.

$$f(\mathbf{Q}, \omega) = f^0(\mathbf{Q}) + f'(\omega) + i f''(\omega)$$

The dispersion corrections are derived by treating atomic electrons as harmonic oscillators. The absorption cross section  $\sigma_a$  is a superposition of oscillators with relative weights, so-called oscillator strengths,  $g(\omega_s)$ , proportional to  $\sigma_a(\omega = \omega_s)$ .



We suppose the electron be subject to the electric field  $E_{in}$  of an incident X-ray beam and to a damping term proportional to the electron velocity  $\Gamma\dot{x}$  which represents dissipation of energy.



The amplitude of the forced oscillations:

$$x_0 = - \left( \frac{e E_0}{m} \right) \frac{1}{(\omega_s^2 - \omega^2 - i \omega \Gamma)}$$

$\Gamma$  = damping factor

$\omega_s$  = resonant frequency

The radiated field  $E_{\text{rad}}$  is proportional to the acceleration of the electron  $\ddot{x}(t-R/c)$  at the detector position  $R$  and at retarded time  $t'=t-R/c$ :

$$\ddot{x}(t - R/c) = -\omega^2 x_0 e^{-i\omega t} e^{i(\omega/c)R}$$

$$\frac{E_{\text{rad}}(R, t)}{E_{\text{in}}} = -r_0 \frac{\omega^2}{(\omega^2 - \omega_s^2 + i \omega \Gamma)} \left( \frac{e^{ikR}}{R} \right)$$

$$f_s \approx -r_0 \left( 1 + \frac{\omega_s^2}{\omega^2 - \omega_s^2 + i \omega \Gamma} \right) = f_0 + f'(\omega) + i f''(\omega)$$

Total scattering length

Thomson term  
(Q dependence)

Frequency-dependent  
refraction index  $n(\omega)$

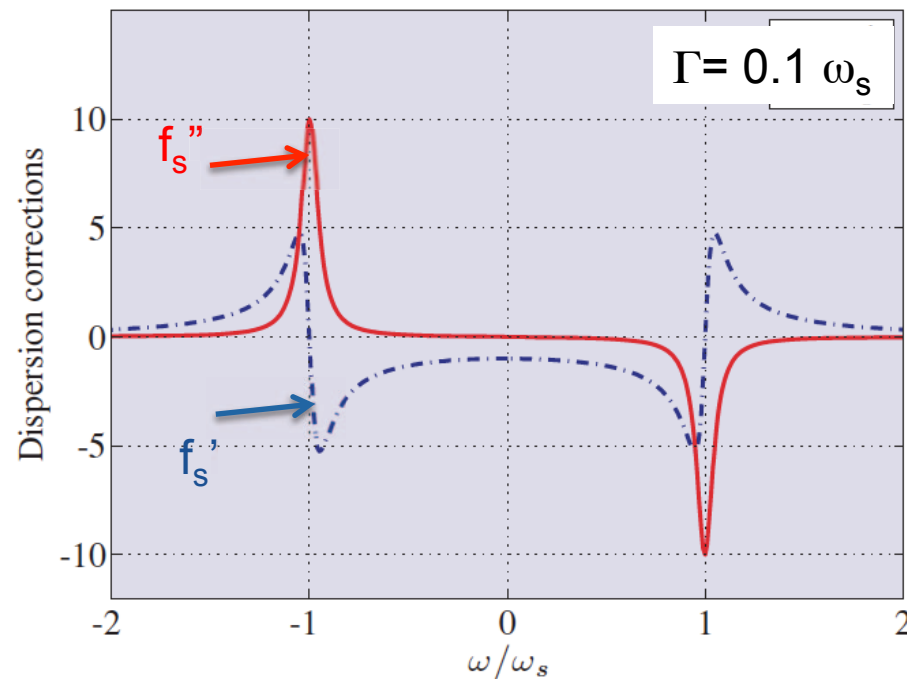
Absorption correction  
(dissipation term)



Real and imaginary part of dispersion correction to the scattering factor

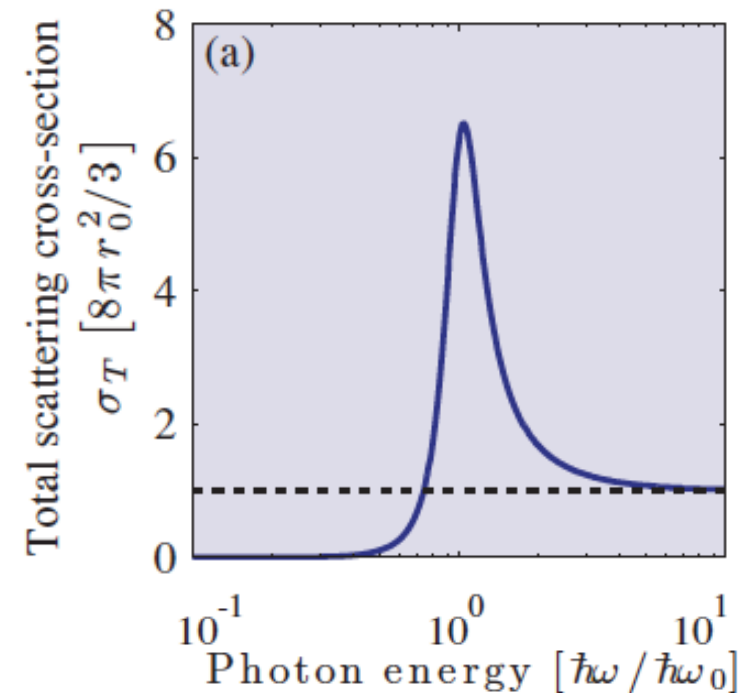
$$f'_s = \frac{\omega_s^2(\omega^2 - \omega_s^2)}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$

$$f''_s = -\frac{\omega_s^2\omega\Gamma}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$



Total scattering cross section for a bound electron

$$\sigma_T = \left(\frac{8\pi}{3}\right) \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2} r_0^2$$



Scattering and refraction are alternative ways to view the same physical phenomenon.

The existence of resonant scattering terms arising from the dispersion corrections can therefore be expected to lead to a frequency dependence of the refractive index  $n$ .

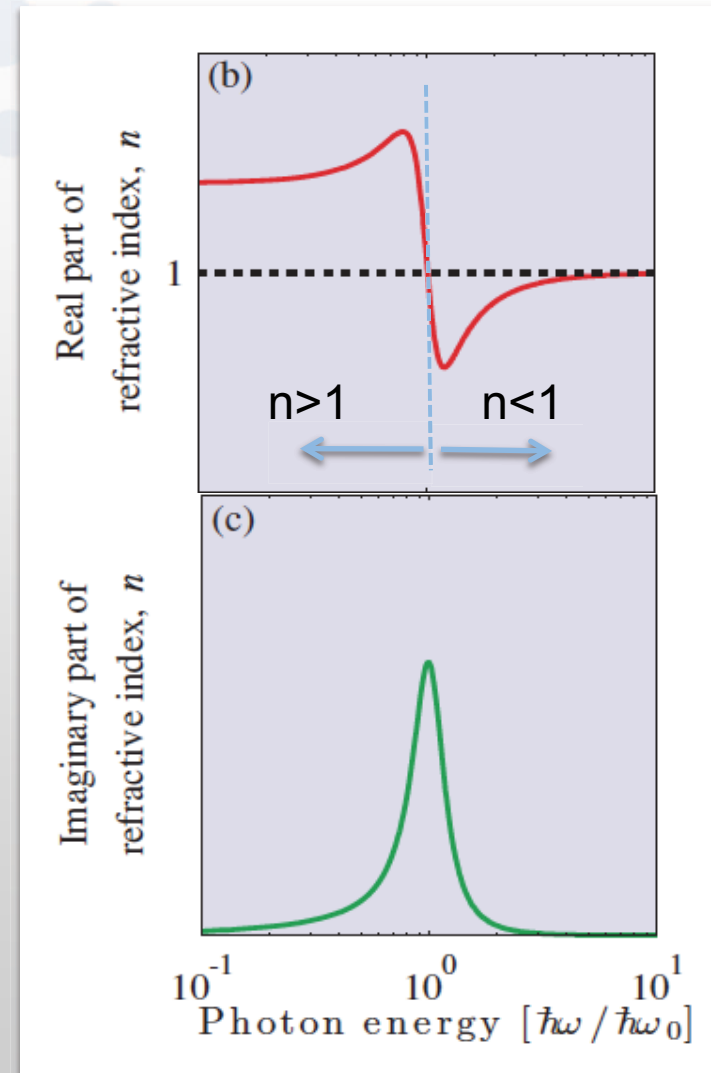
$$n^2 = 1 + \left( \frac{e^2 \rho}{\epsilon_0 m} \right) \frac{1}{(\omega_s^2 - \omega^2 - i \omega \Gamma)}$$

For  $\omega \ll \omega_s \Rightarrow n > 1$  visible light

For  $\omega \gg \omega_s \Rightarrow n < 1$  x-rays

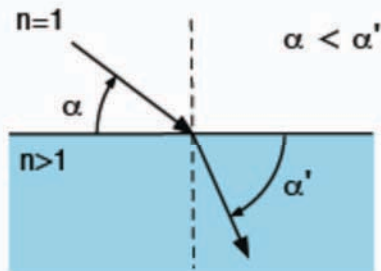
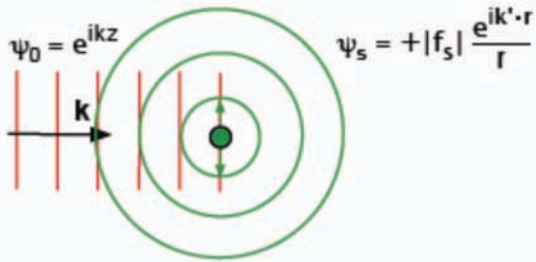
Notice that if  $\omega \gg \omega_s \gg \Gamma$

$$n \approx 1 - \frac{1}{2} \frac{e^2 \rho}{\epsilon_0 m \omega^2} = 1 - \frac{2\pi r_0}{k^2}$$

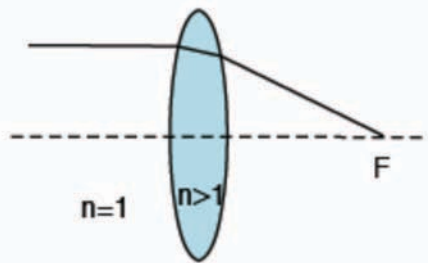


Snell law:  $n_1 \cos \alpha = n_2 \cos \alpha'$

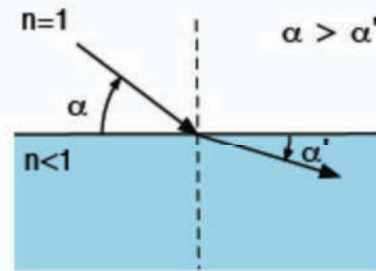
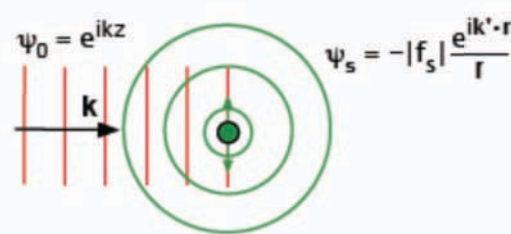
### Visible light



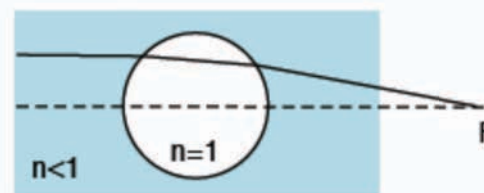
### Optic lenses



### X-rays



### X-rays lenses



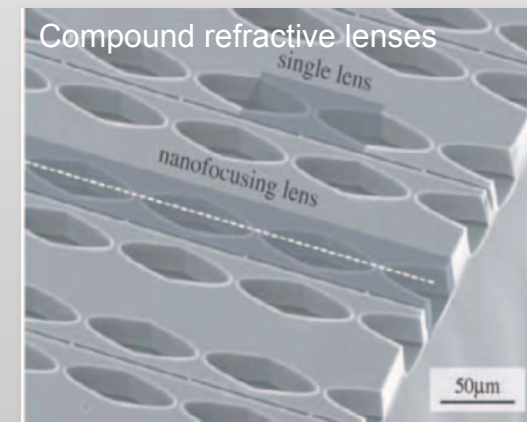
Refraction index for X-rays:

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

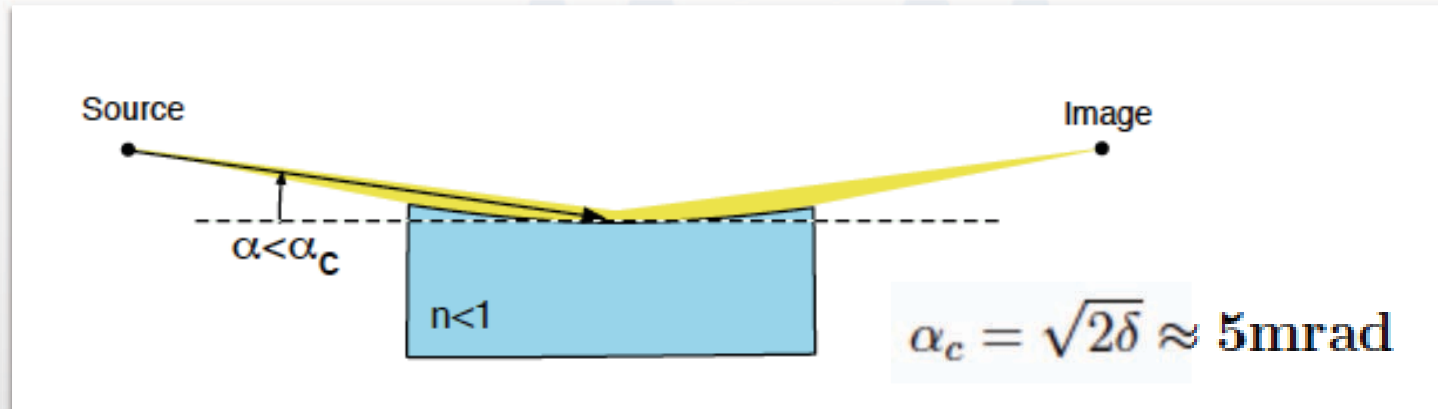
$$\delta(\text{air}) \sim 10^{-8}$$

$$\delta(\text{solids}) \sim 10^{-5}$$

$$\beta \sim 10^{-8} \ll \delta$$



The critical angle for the total reflection:



High quality mirrors are required for x-rays focusing and a large radius tangential focusing

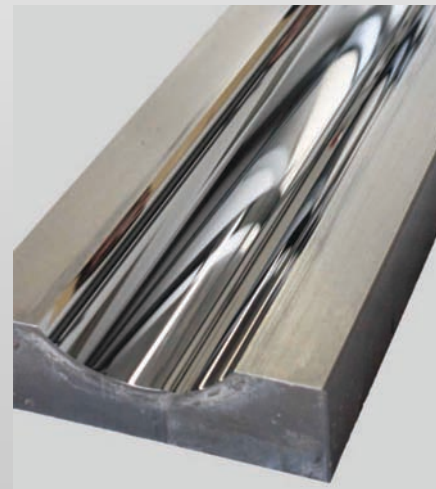
Ex: silicon mirror with toroidal shape

Distance from source  $p=76\text{m}$ ,

Distance mirror object  $q=26\text{m}$

$\theta=2.7 \text{ mrad}$

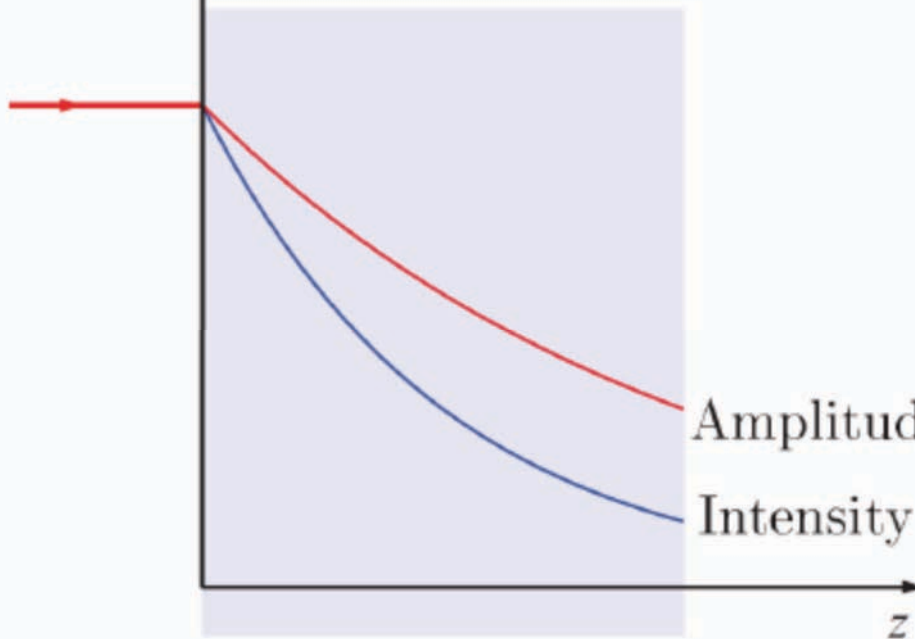
$\rho_{\text{sagittal}}=27 \text{ cm}$   $\rho_{\text{tang}}=27 \text{ km}$



The attenuation of x-rays in a medium depends from the imaginary part  $\beta$  of refraction index:

$$e^{ikz} \quad e^{inkz} = e^{i(1-\delta)kz} e^{-\beta kz}$$

$$\beta = \frac{\mu}{2k}$$



Including dispersion corrections:

$$n \equiv 1 - \frac{2\pi \rho_a r_0}{k^2} \{f^0(0) + f' + i f''\}$$

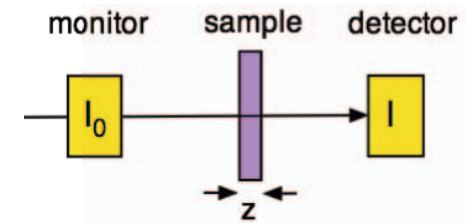
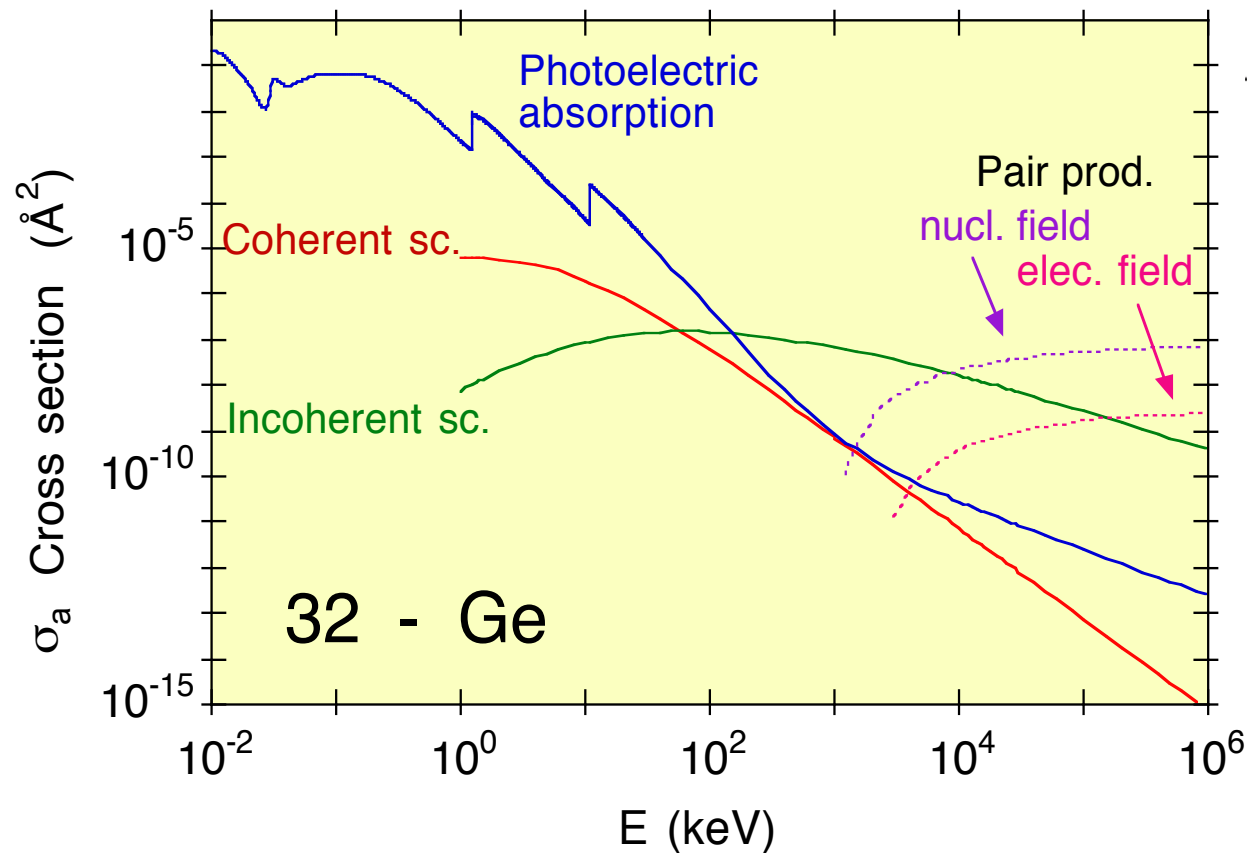
and:

$$f'' = - \left( \frac{k}{4\pi r_0} \right) \sigma_a$$

Optical theorem

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

The absorption cross section can be measured by a transmission method.

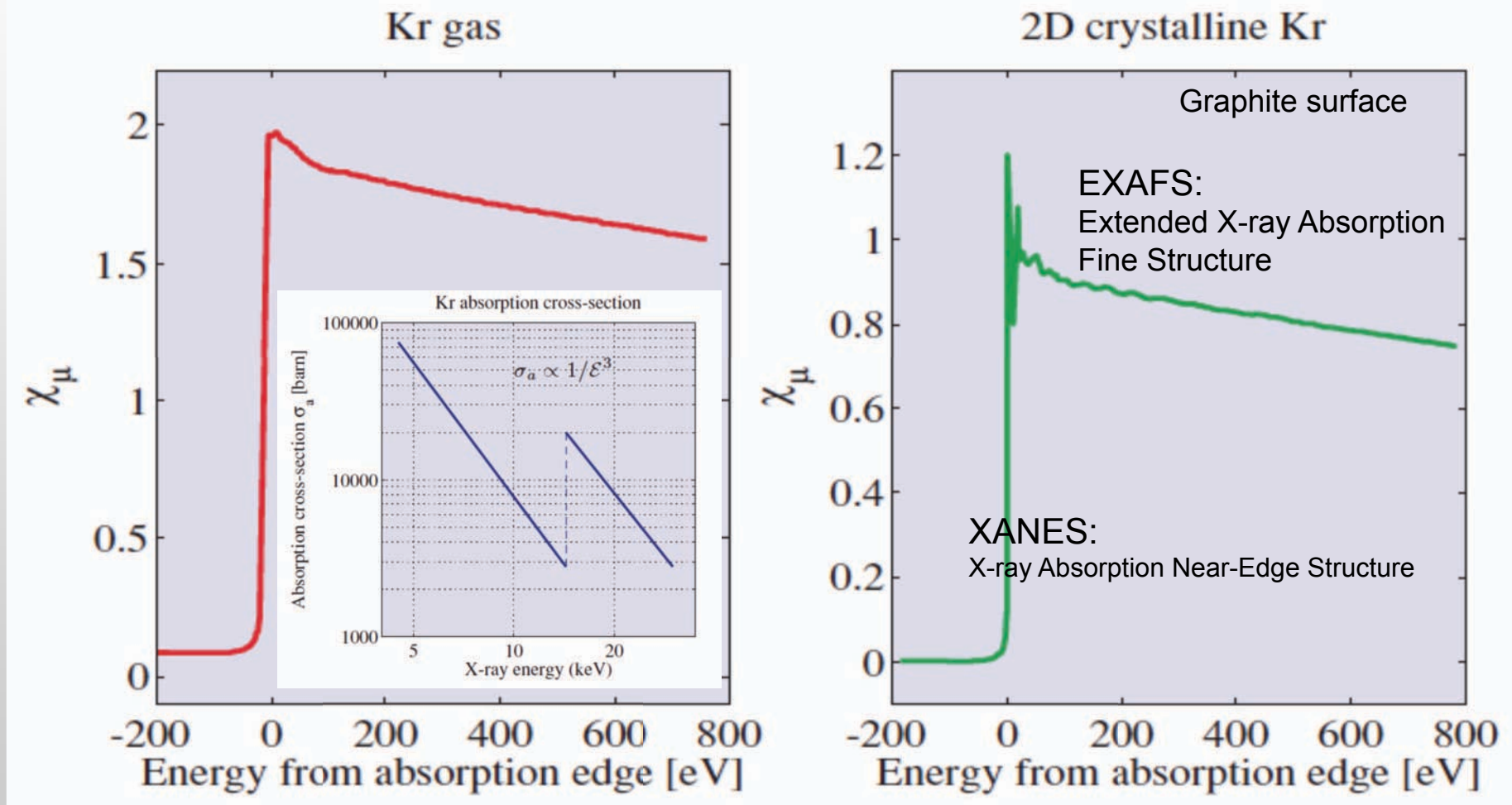


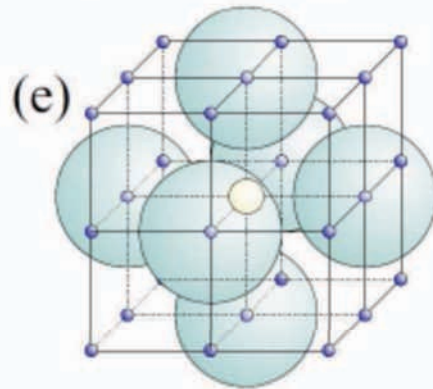
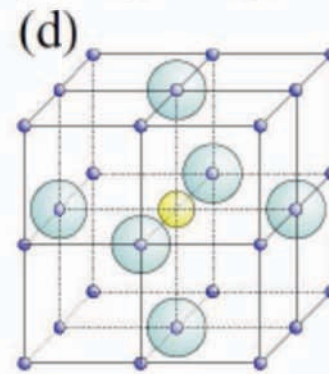
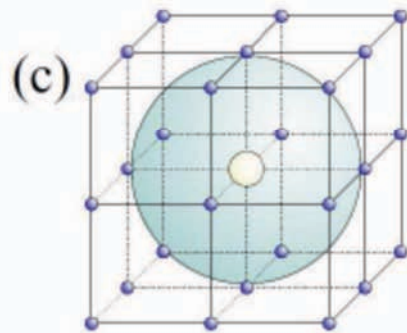
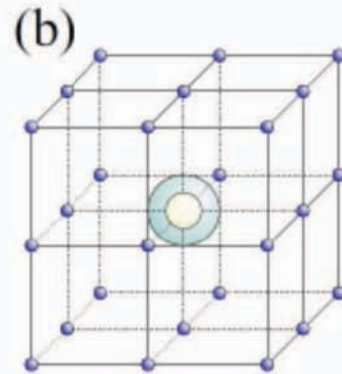
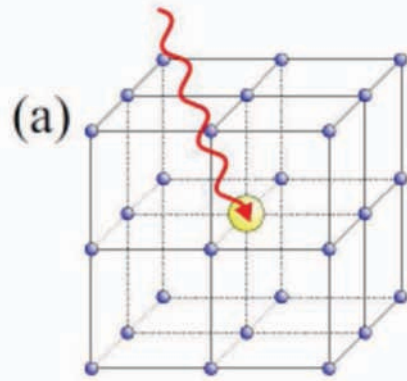
$$T = \frac{I}{I_0} = e^{-\mu z}$$

Absorption coefficient

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

The transitions from core electron levels to empty states produce in the absorption spectrum simple threshold structures in the case of isolated atoms or modulated structures well above the threshold when the atom is embedded in a crystalline environment.





$$\chi(q(\mathcal{E})) = \frac{\mu_{\chi}(\mathcal{E}) - \mu_0(\mathcal{E})}{\mu_0(\mathcal{E})}$$

$$\frac{\hbar^2 q^2}{2m} = \mathcal{E} - \hbar\omega_K$$

In transmission:

$$T = \frac{I_1}{I_0} = e^{-\mu(\mathcal{E})d}$$

$$\begin{aligned} \mu(\mathcal{E}) &= \mu_A(\mathcal{E}) + \mu_{\chi}(\mathcal{E}) \\ &= \mu_A(\mathcal{E}) + \mu_0(\mathcal{E}) [1 + \chi(q)] \end{aligned}$$

In fluorescence:

$$I_f = I_0 \epsilon \left( \frac{\Delta\Omega}{4\pi} \right) \frac{\mu_{\chi}(\mathcal{E})}{\mu(\mathcal{E}) + \mu(\mathcal{E}_f)} \left[ 1 - e^{-(\mu(\mathcal{E}) + \mu(\mathcal{E}_f))d} \right]$$

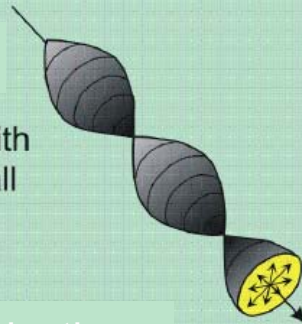


Direct Sun light



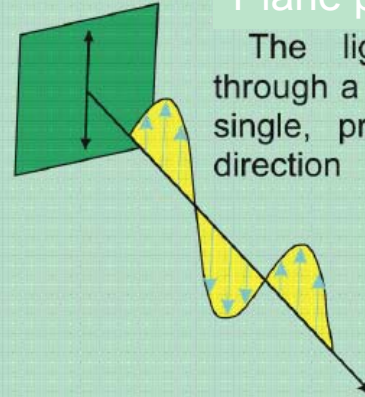
Unpolarized

Single light ray with light vibrating in all directions.



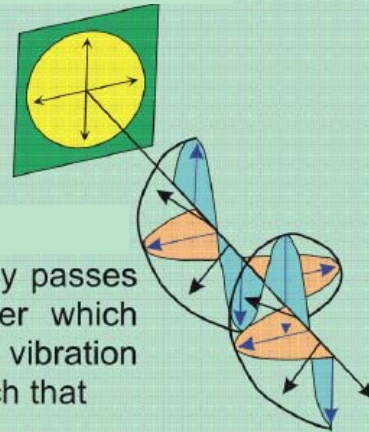
Plane polarized

The light ray passes through a filter which has a single, preferred vibration direction

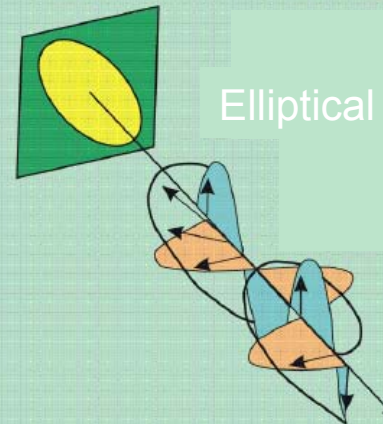


Circular polarization

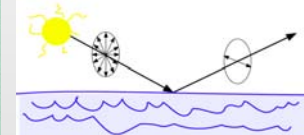
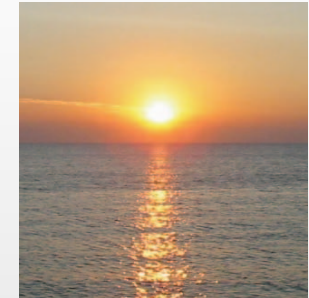
The light ray passes through a filter which has two vibration directions, such that  $\Delta = 1/4\lambda$ .



Elliptical polarization



Reflected Sun light



Birfringence in calcite



## Linear dichroism

Produced by the preferential absorption of one of the two orthogonal photon polarization



Linearly oriented polymers  
When the electric field is parallel to the preferential molecular axis, it is absorbed

## Circular dichroism

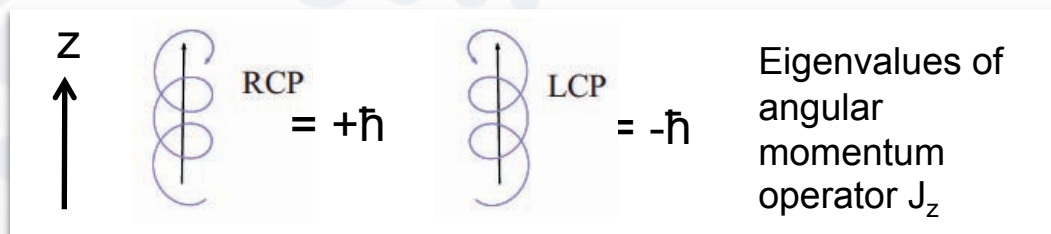
Produced by the preferential absorption of one of the two circular photon polarization



Combination of  $\lambda/4$  and linear polarized filters have the different effect on circular polarization.  
Circular dichroism is found also in chiral molecules which select only one circular polarization (ex. sugar)

Quantum description of a circular polarised photon beam:

RCP and LCP eigenstates of  $J_z$

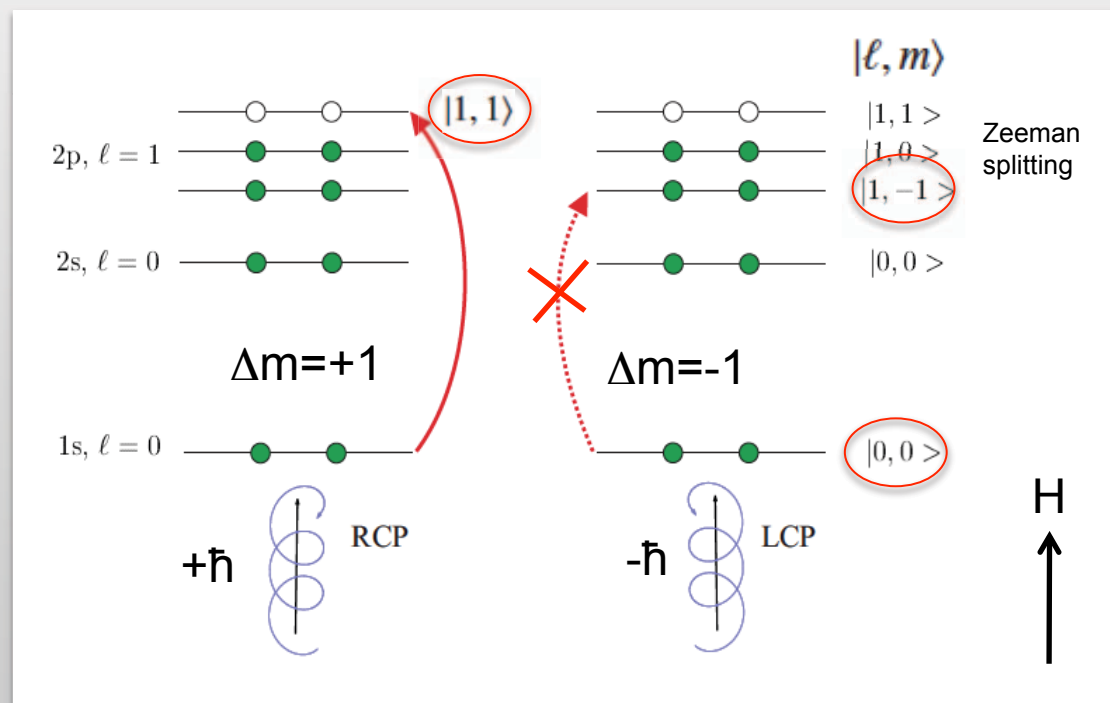


The sum rule for the conservation of angular momentum in electronic transition produces a difference in the absorption of RCP and LCP photons.

Ex.: Dipole electric transitions in Oxygen

selection rule:  $\Delta l \pm 1$   
(odd function for coordinate exch.)

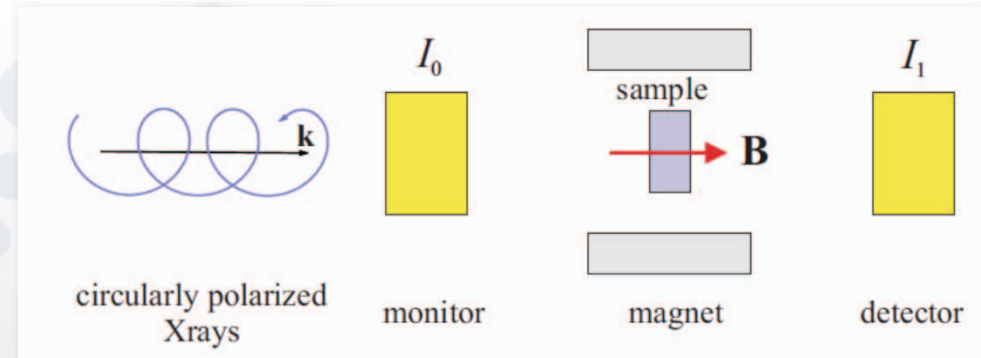
Transition allowed:  
 $\Delta m = +1$  for RCP  
 $\Delta m = -1$  for LCP



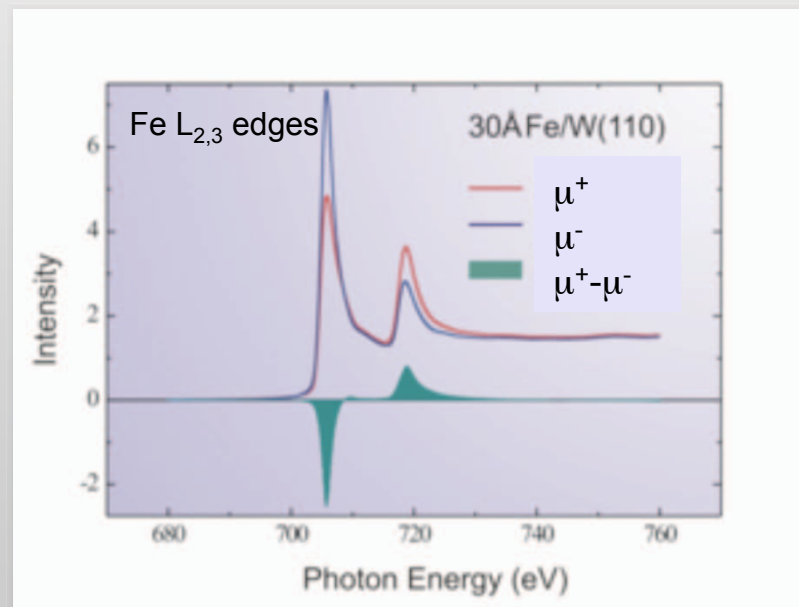
Absorption coefficients

$$\mu^+(E) = \left(\frac{1}{d}\right) \ln \left(\frac{I_0^+(E)}{I_1^+(E)}\right)$$

$$\mu^-(E) = \left(\frac{1}{d}\right) \ln \left(\frac{I_0^-(E)}{I_1^-(E)}\right)$$



The difference between  $\Delta\mu = \mu^+ - \mu^-$  is enhanced across the absorption edge because the electronic transitions to final states are strongly magnetically polarized



Thole et al., Phys. Rev. Lett. 68 (1992) 1943; Carra et al., Phys. Rev. Lett. 70 (1993) 694

## Orbital and spin magnetic moment determination in 3d electron systems

$$m_{\text{orb}} [\mu_B/\text{atom}] = -\frac{4q(10 - n_{3d})}{r}$$

$$m_{\text{spin}} [\mu_B/\text{atom}] \approx -\frac{(6p - 4q)(10 - n_{3d})}{r}$$

$$p = \int_{L_{III}} (\mu^+ - \mu^-) d\mathcal{E}$$

$$q = \int_{L_{III}+L_{II}} (\mu^+ - \mu^-) d\mathcal{E}$$

$$r = \int_{L_{III}+L_{II}} (\mu^+ + \mu^-) d\mathcal{E}$$

