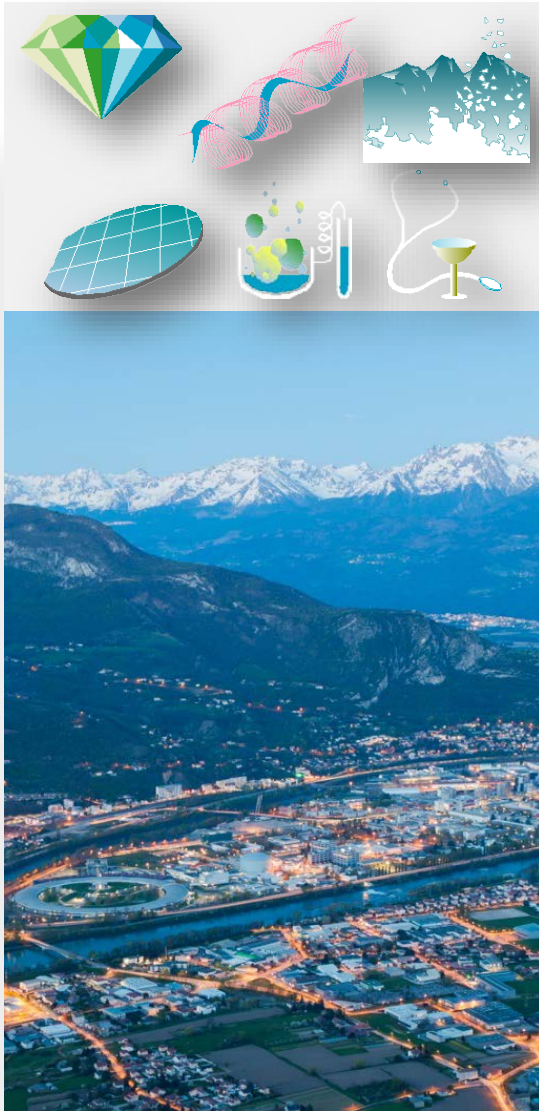


X-rays and their interaction with matter

Luigi Paolasini

European Synchrotron Radiation Facility
paolasini@esrf.eu





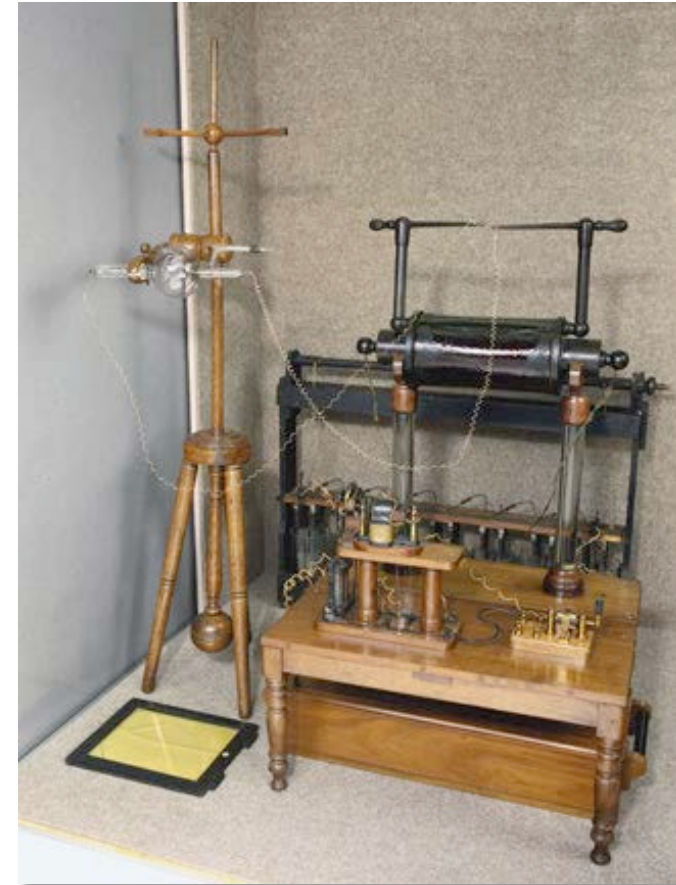
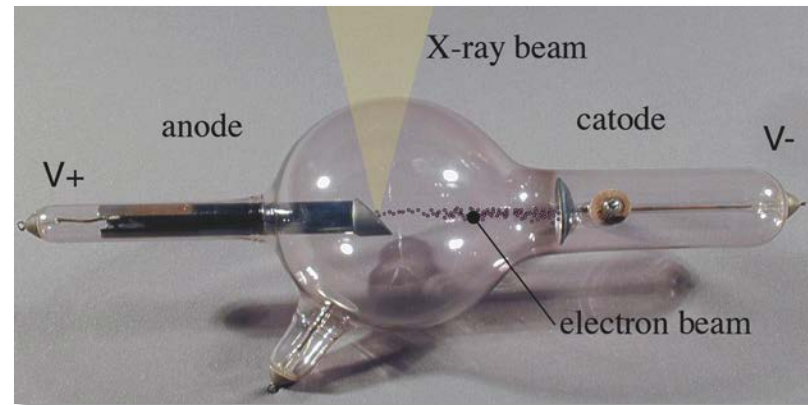
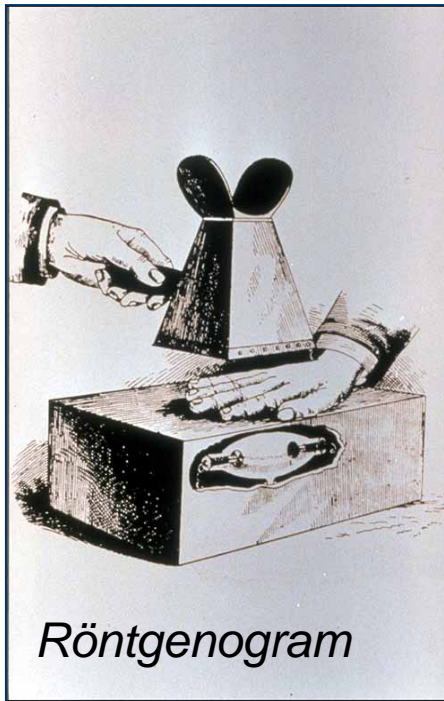
“X-rays and their interaction with matter”

- Waves and photons
- Elastic and inelastic scattering
- Absorption spectroscopies
- Optical properties

X-RAY DISCOVERY: W.C. RÖNTGEN, 1895

Röntgen discovered a penetrating form of electromagnetic radiation able to pass through the human body: the X-rays.

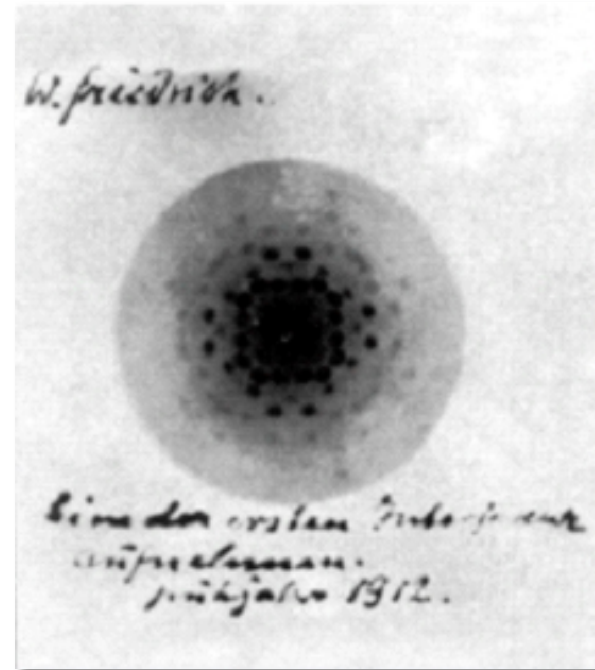
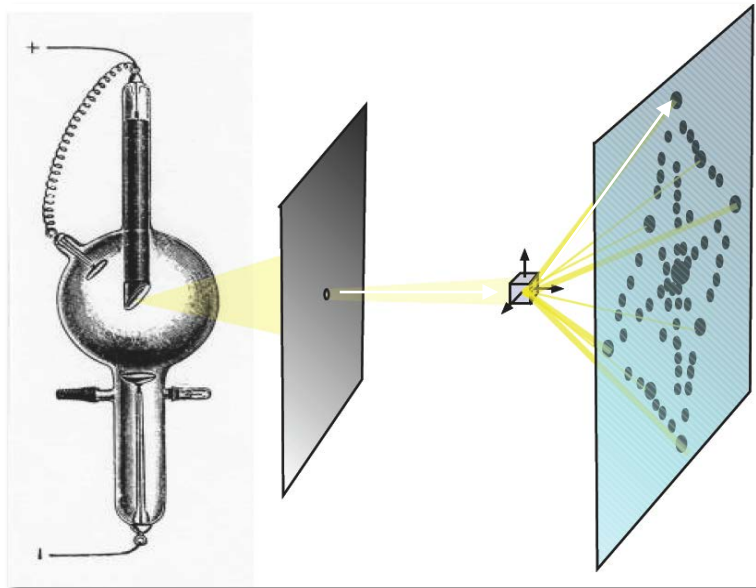
X-rays are produced by collision of electrons with a metal target (kinetic energy loss, “bremstralung”)



CRYSTAL DIFFRACTION: MAX VON LAUE, 1912

X-rays are electromagnetic waves:

- The x-ray wavelengths are comparable with the interatomic distances and molecular bonds.
- Typical interference x-ray patterns when pass through a periodic arrangement of atoms, like in a crystal, and reveal their crystallographic symmetries.

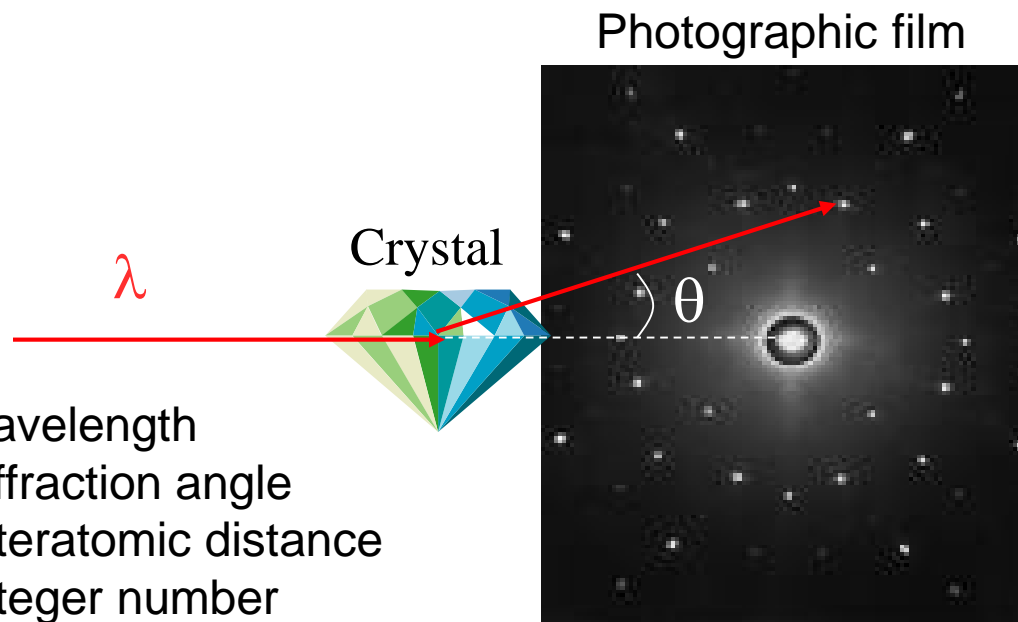


THEORY OF X-RAYS DIFFRACTION: BRAGG LAW, 1913

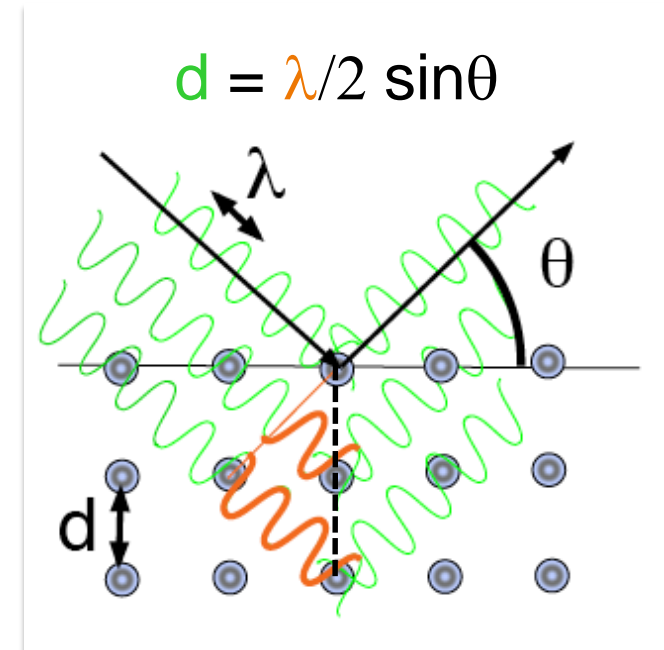
The interference X-ray pattern contains the signature of the periodic arrangement of atoms in a crystals.

The Bragg's law define the relation between interatomic distances d and scattering angle θ

$$\text{Bragg Law: } 2d \sin\theta = n\lambda$$



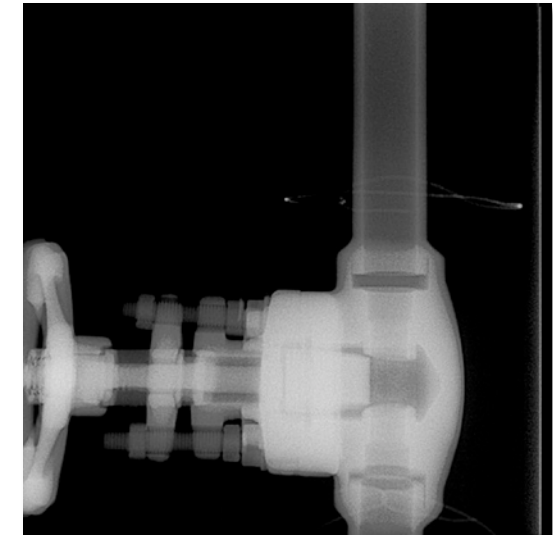
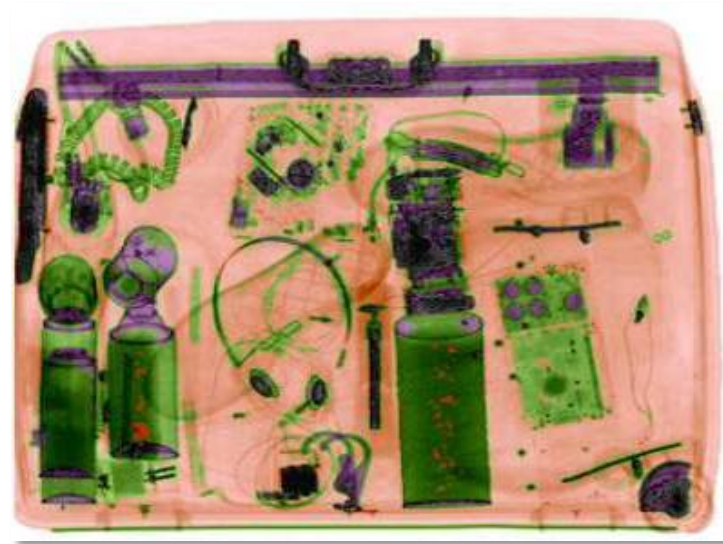
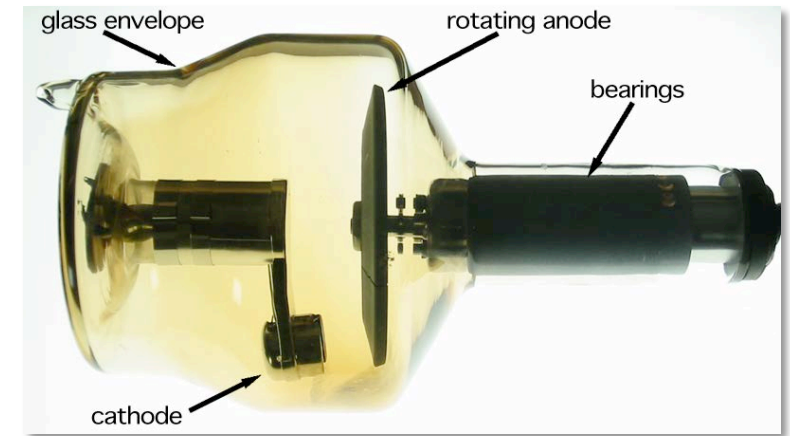
- λ : wavelength
- θ : diffraction angle
- d : interatomic distance
- n : integer number



X-RAY TUBES: ROTATING ANODE

Today powerful x-rays sources can be obtained by rotating anode x-ray tubes.

X-ray tubes are also used in CAT scanners, airport luggage scanners, X-ray crystallography, and for industrial inspection.

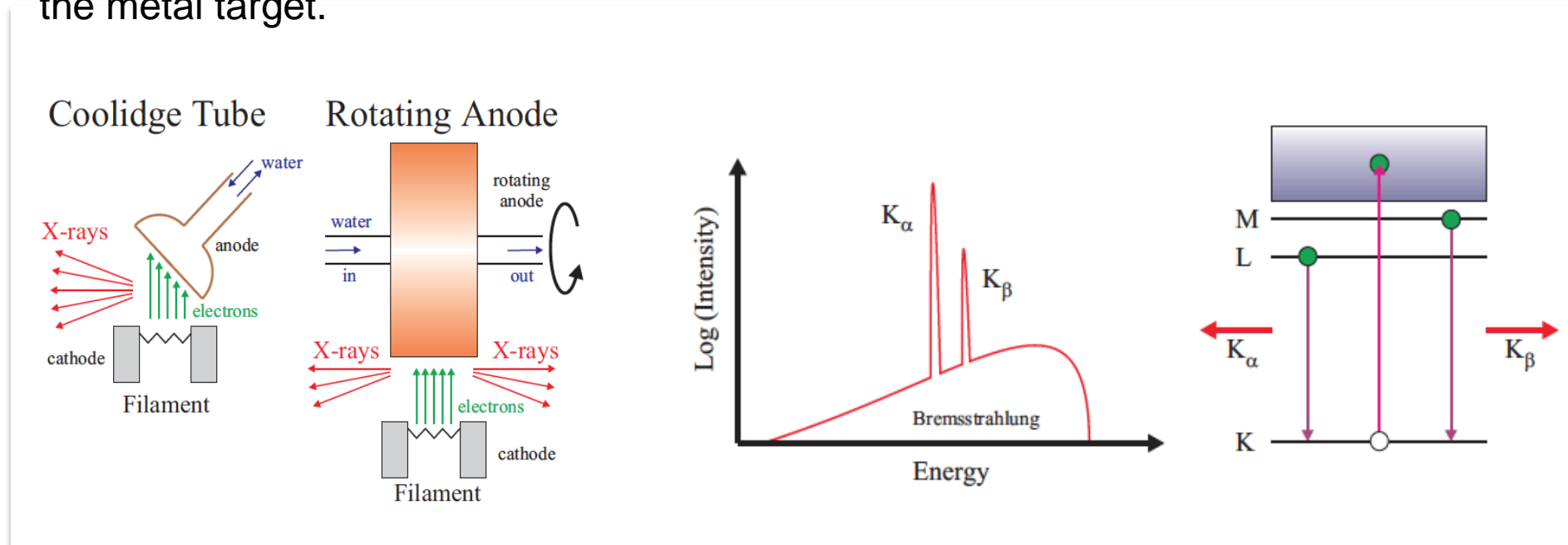


FROM COOLIDGE TUBE TO ROTATING ANODE.

W.D. Coolidge's tube from General Electric developed in 1912 served as the standard X-ray tube for many decades until the advent of rotating anode generators.

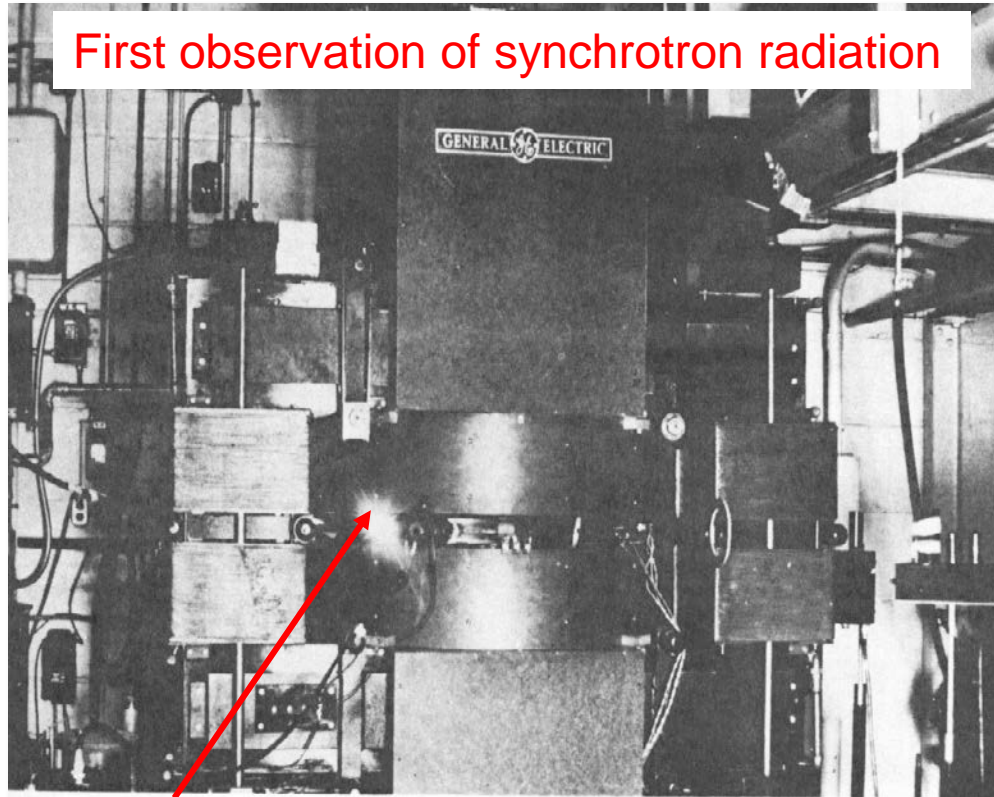
The spectrum of X-rays generated from electrons impinging on a metal anode has two distinct components:

- Only 1% of the incident energy is emitted in the form of x-rays
- Bremsstrahlung radiation : a continuous component
- Sharp radiations with a characteristic energy emission K_α and K_β of the metal target.



DISCOVERY OF SYNCROTRON RADIATION : GENERAL ELECTRIC 1947

Electromagnetic radiation emitted when **charge particles** moving at **ultra-relativistic energies** are forced to change direction under the action of a magnetic field.

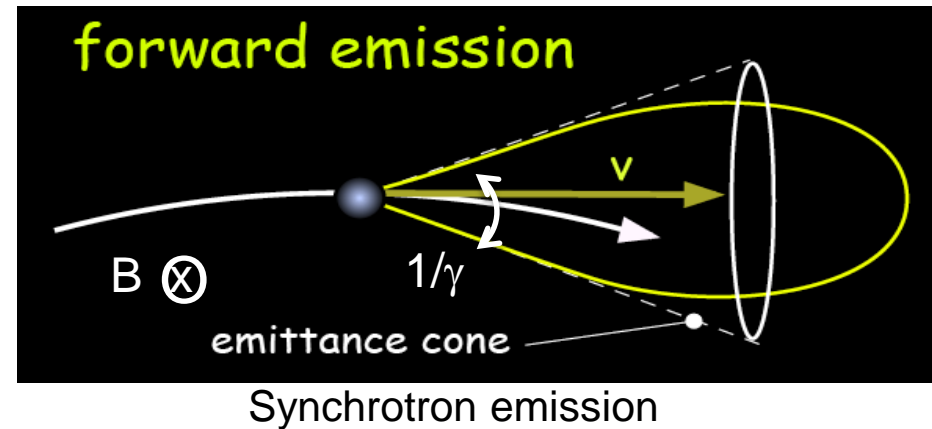


Visible light emission discovered in a 70-MeV betatron at General Electric in 1947.

$$E \gg m_e c^2 \sim 0.511 \text{ MeV}$$

$$\gamma = E/m_e c^2 \gg 1$$

$$\gamma \sim 1957 E[\text{GeV}]$$



X-RAYS LARGE SCALE FACILITIES

SYNCHROTRONS :

the electrons circulate in a close orbit

FREE ELECTRON LASERS:

the electrons travel in linear accelerators



X-RAYS ARE ELECTROMAGNETIC WAVES

The electromagnetic field generated by the electrons is described by the electric \mathbf{E} and magnetic \mathbf{B} in term of scalar Φ and vector \mathbf{A} potential:

$$\vec{\mathbf{B}} = \nabla \times \vec{\mathbf{A}}$$

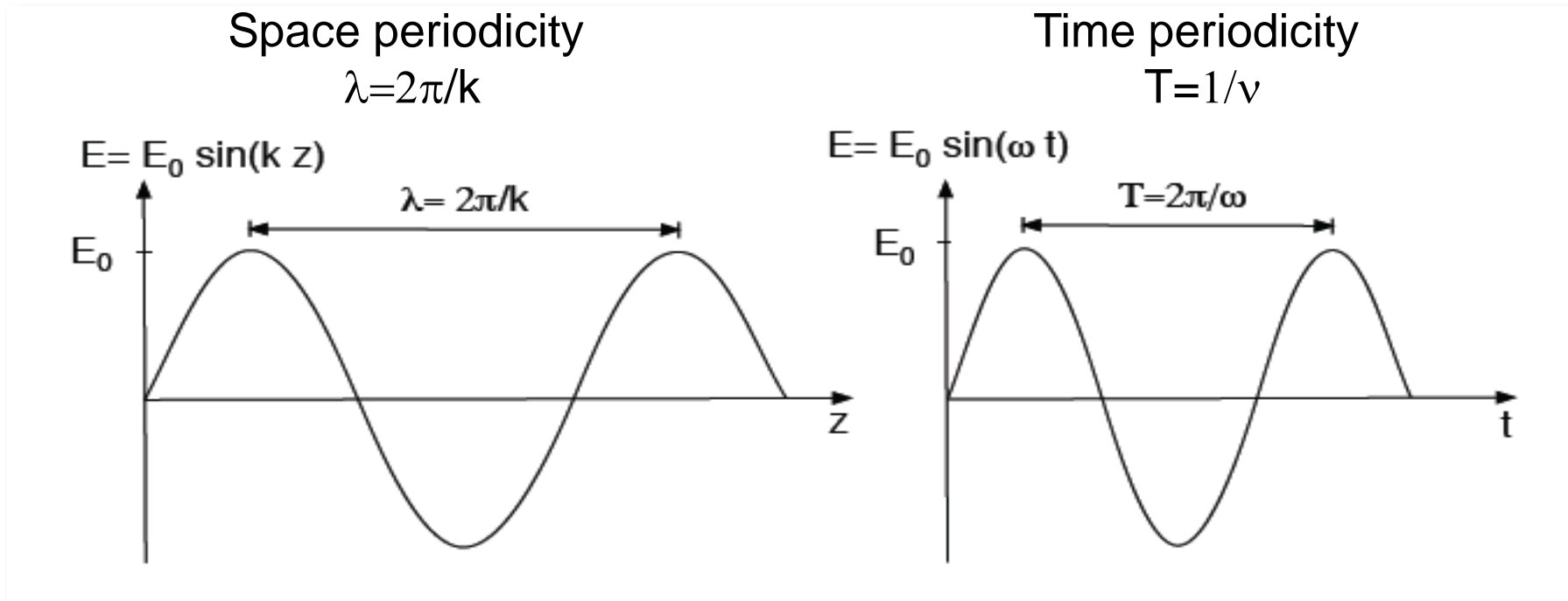
$$\vec{\mathbf{E}} = -\nabla\Phi - \frac{1}{c} \frac{\partial \vec{\mathbf{A}}}{\partial t}$$

*Maxwell equations
(Coulomb gauge)*

$$\mathbf{E} = \mathbf{E}_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$

$$\mathbf{B} = \mathbf{B}_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$

$$\mathbf{A} = \mathbf{A}_0 e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$

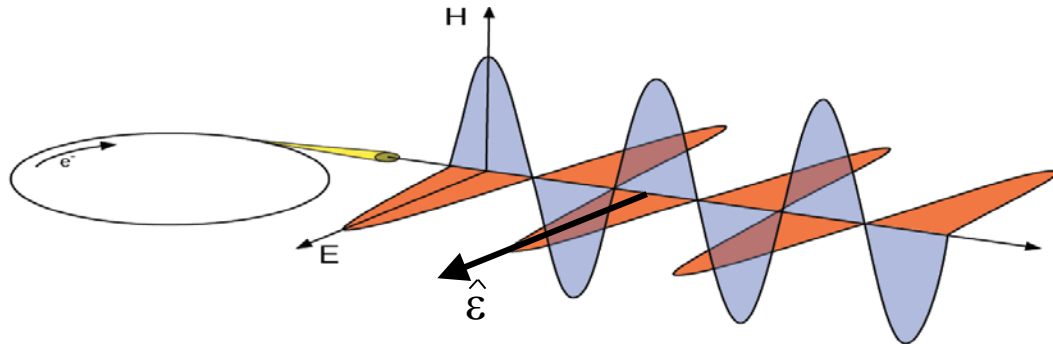


X-RAYS POLARISATIONS

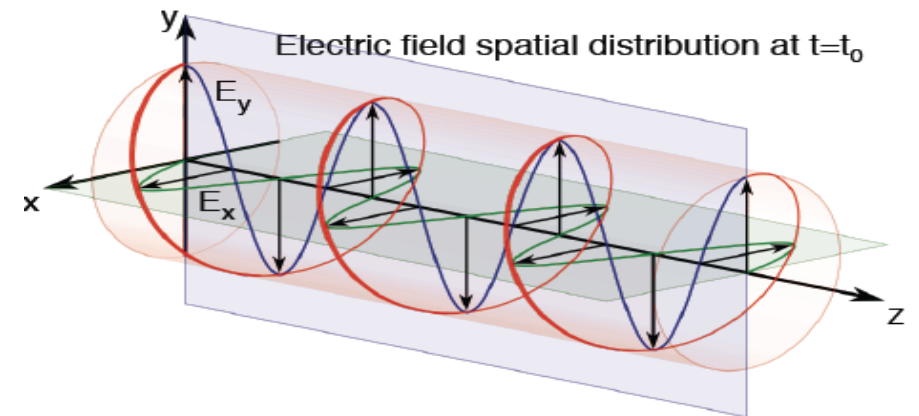
The X-rays delivered by the insertion devices (bending magnets or undulators) is a transverse polarized electromagnetic wave, with the polarization vector $\hat{\epsilon}$ parallel to the electric field \mathbf{E} .
Some particular insertion devices can also deliver circular polarization (ex. helical undulators, phase plates)

Linear transverse EM wave

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



Circular transverse EM wave



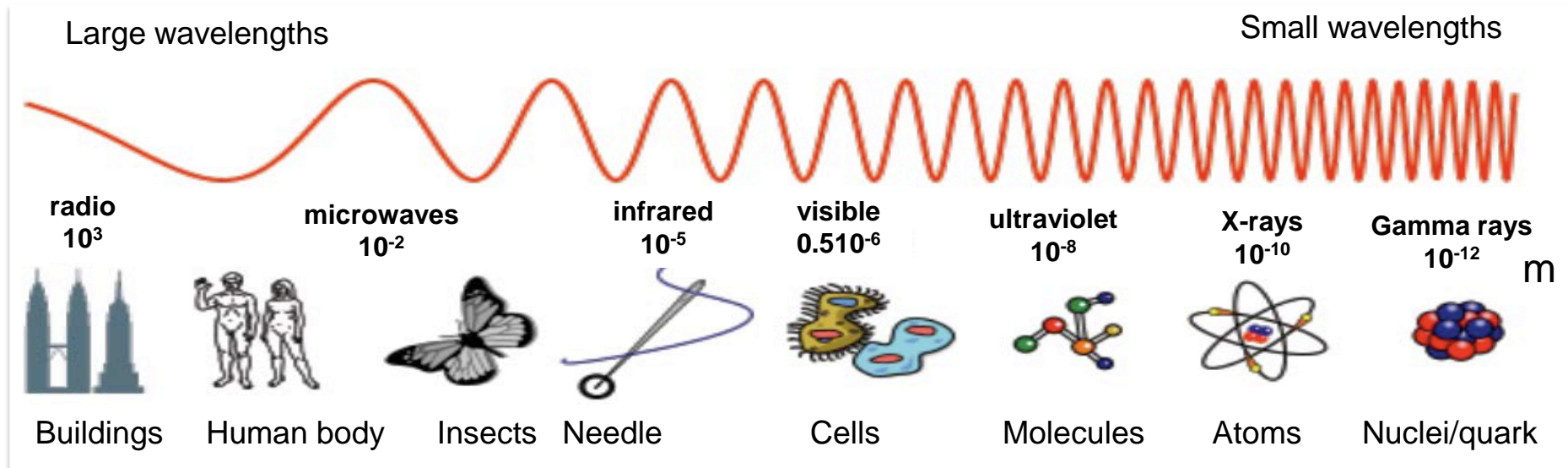
$$E_x = E_{x0} \cos\left[2\pi\left(\frac{z}{\lambda} - \frac{t}{T}\right)\right]$$

$$E_y = E_{y0} \sin\left[2\pi\left(\frac{z}{\lambda} - \frac{t}{T}\right)\right]$$

- $E_{x0} = \pm E_{y0}$ Circular polarisation (right=+, left=-)
- $E_{x0} = 0$ or $E_{y0} = 0$ Linear polarization
- $E_{x0} \neq E_{y0} \neq 0$ Elliptical polarization

THE ELECTROMAGNETIC SPECTRUM

The electromagnetic radiation is generated by the accelerated charged particles (electron, protons ...)



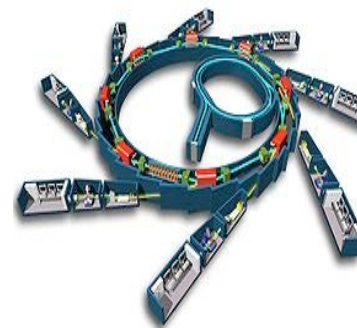
Radio waves



Radar



Microscopes



Synchrotrons



Large accelerators

ULTRA SMALL

$$\mathcal{E}[\text{keV}] = \frac{hc}{\lambda} = \frac{12.398}{\lambda[\text{\AA}]}$$

Planck's constant $h = 4.135 \times 10^{15} \text{ eV s}$

ex. $1 \text{ \AA} = 0.1 \text{ nm} @ 12.398 \text{ keV}$

Hard X-rays

1.2 MeV - 2.5 keV

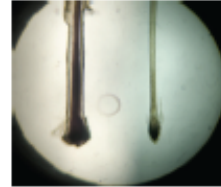
$\sim 0.001 \div 0.5 \text{ [nm]}$

Soft X-rays

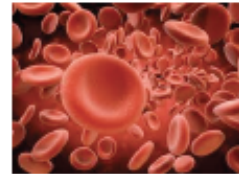
2.5 keV - 100 eV

$\sim 0.5 \div 12 \text{ [nm]}$

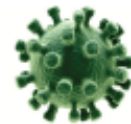
Nature



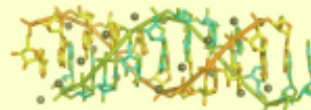
Human hair $\sim 30 \mu\text{m}$



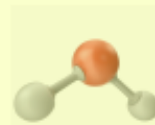
Red blood cells $\sim 5 \mu\text{m}$



Virus $\sim 200 \text{ nm}$



DNA helix width $\sim 3 \text{ nm}$



Water molecule $\sim 275 \text{ pm}$

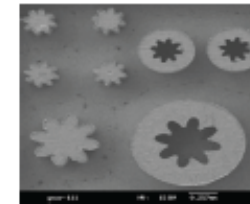
Man made

10^{-3} m 1 mm



Head of a pin
 $\sim 1 \text{ mm}$

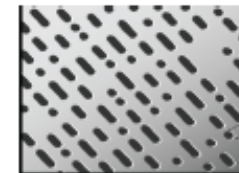
100 μm



Micro gears
diameters
 $\sim 10\text{-}100 \mu\text{m}$

10 μm

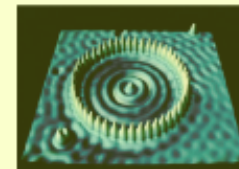
10^{-6} m 1 μm



DVD tracks
 $\sim 400\text{-}700 \text{ nm}$

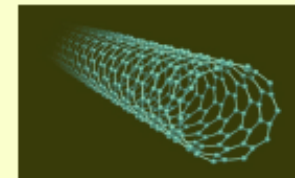
100 nm

10 nm



Atomic corral
 $\sim 14 \text{ nm}$

10^{-9} m 1 nm



carbon nanotubes
 $\sim 2 \text{ nm}$

100 pm

ULTRA FAST

10keV X-rays

$$2.4 \times 10^{18} \text{ Hz} = 2.4 \text{ exa Hz}$$

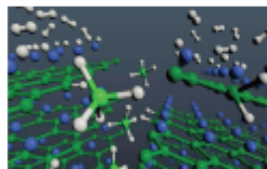
$$T = 41 \times 10^{-3} \text{ fs} = 41 \text{ attosecond}$$

$$\lambda = 12.5 \text{ nm} = 1.25 \text{ \AA}$$

Pulse duration ESRF
20 ps

Pulse duration X-FEL (theory)
4.5 fs

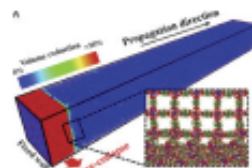
Nature



Hydrogen transfer time in molecules $\sim 1 \text{ ns}$



Spin Larmor precession in 1T field $\sim 10 \text{ ps}$



Shock wave propagates by 1 atom in $\sim 100 \text{ fs}$



Water dissociates in $\sim 10 \text{ fs}$



Bohr period of a valence electron $\sim 1 \text{ fs}$

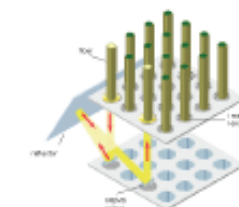
Man made



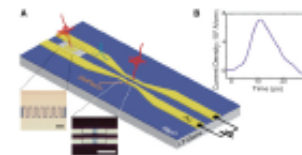
Computing time per bit $\sim 1 \text{ ns}$



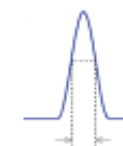
Magnetic recording time per bit $\sim 2 \text{ ns}$



Optical network switching time per bit $\sim 100 \text{ ps}$



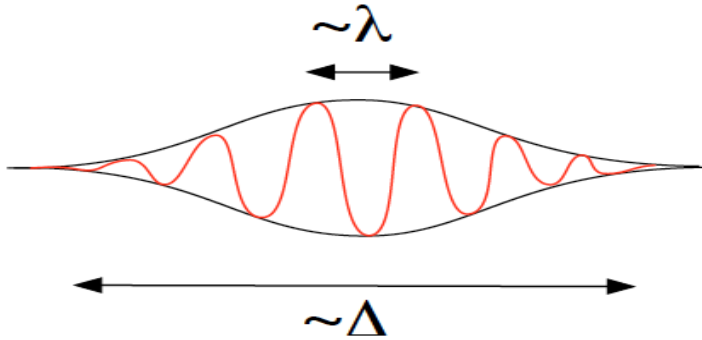
Laser pulsed current switch $\sim 10 \text{ ps}$



Shortest laser pulse $\sim 1 \text{ fs}$

WAVE-PARTICLE DUALITY

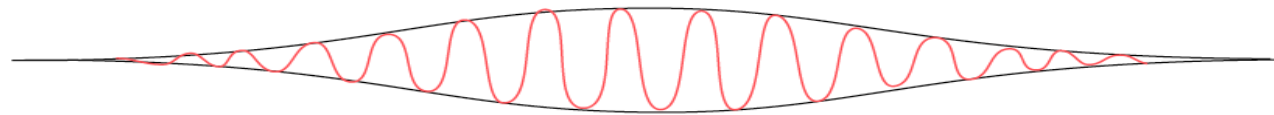
Description of the behaviour of a quantum-scale objects.



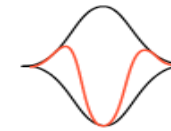
Heisenberg uncertainty principle:
Cannot define both Δ and λ to an arbitrary accuracy

Oscillations \rightarrow wave
Envelope \rightarrow particle localization

Wave: $\Delta \gg \lambda$



particle: $\Delta \ll \lambda$



Decreasing Δ to define better the position, but we lose information on λ

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

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

where

h = Planck's constant
 ν = frequency
 k = wavevector

Assumption of quantum mechanics:

- (i) Particles are 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 (spatial part):

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

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

1 particle per unit volume everywhere!

Spherical wave:

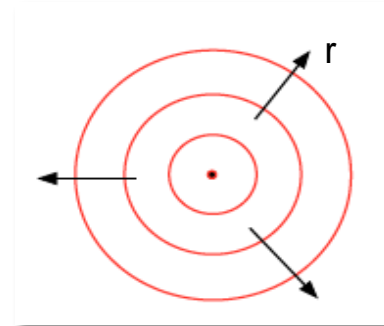
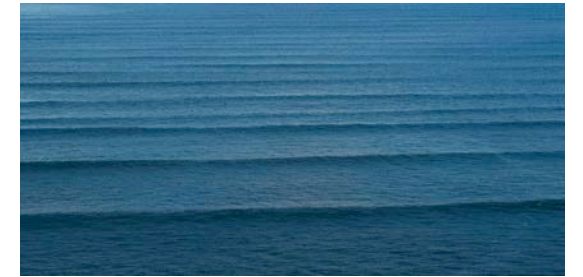
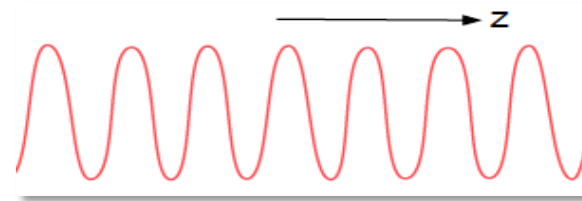
$$\psi(\underline{r}) = b/r e^{ikr}$$

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

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

Flux of particles

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



TOTAL SCATTERING CROSS SECTION

Total cross section: Effective area viewed by scattering particles!

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

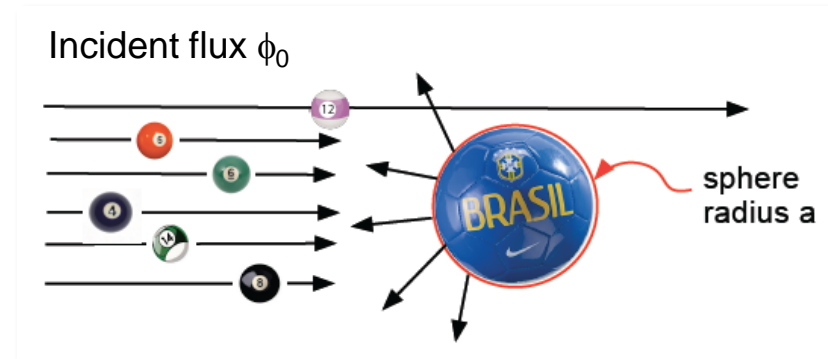
Classical case:

no. particles scattered per second = $\phi_0 \times \pi a^2$

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

Particles x unit area x sec.

Cross-sectional area of sphere



Quantum case:

Incident wave

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

Incident flux

$$\phi_0 = |\psi_0|^2 v = v$$

Scattered wave

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

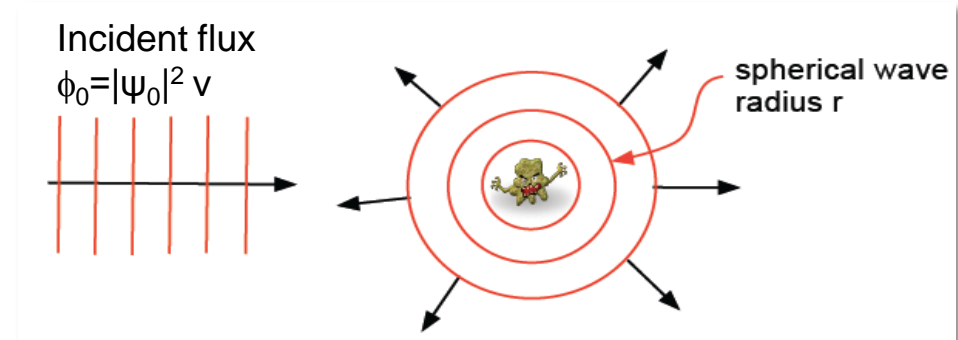
Scattered flux

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

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

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

b = scattering length



DIFFERENTIAL SCATTERING CROSS SECTION

Definition: differential scattering cross section

$$\frac{d\sigma}{d\Omega} = \frac{\text{Number of particles scattered into solid angle } d\Omega \text{ per sec.}}{\text{incident flux} \times d\Omega}$$

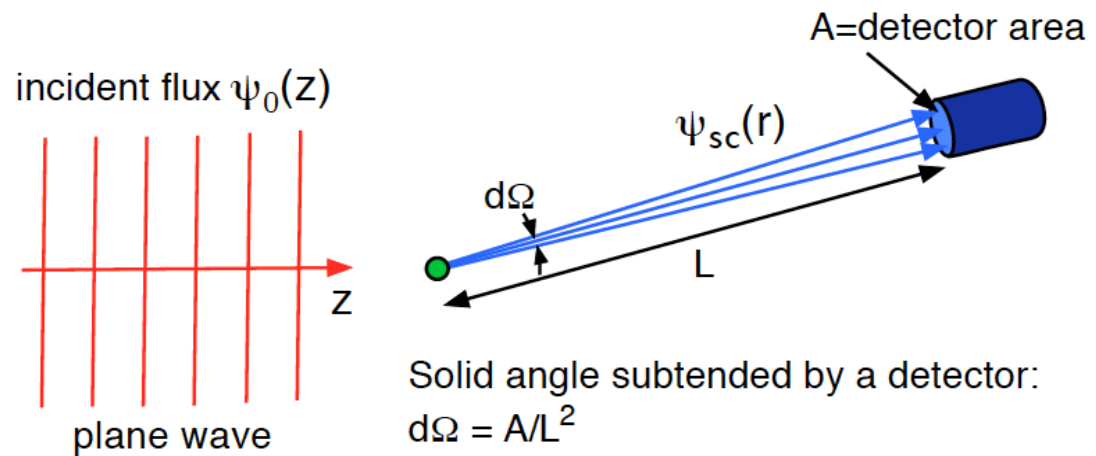
Solid angle subtended by the detector:

$$\Delta\Omega = A/L^2$$

No. particles detected per sec.:

$$d\sigma/d\Omega = (|\psi_{sc}|^2 v \times A) / (|\psi_0|^2 v d\Omega)$$

$$|\psi_{sc}|^2 = b^2/L^2 \quad \text{Detector area}$$



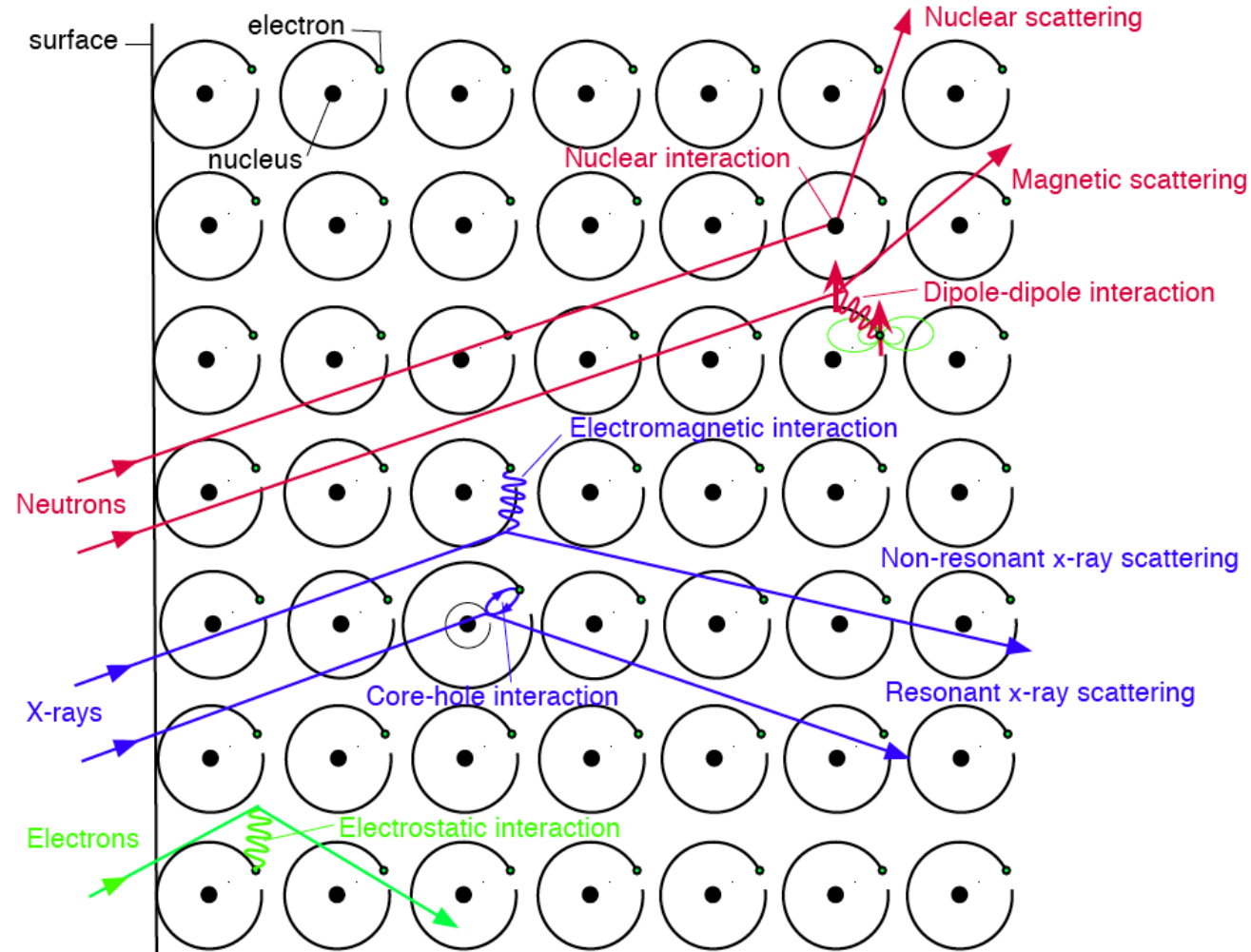
$$\frac{d\sigma}{d\Omega} = \frac{|\psi_{sc}|^2}{|\psi_0|^2} L^2 = b^2 = \frac{\sigma}{4\pi}$$

(barns/steradian)

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

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

The scattering length b depends from the type of interaction potential with the scattering probes

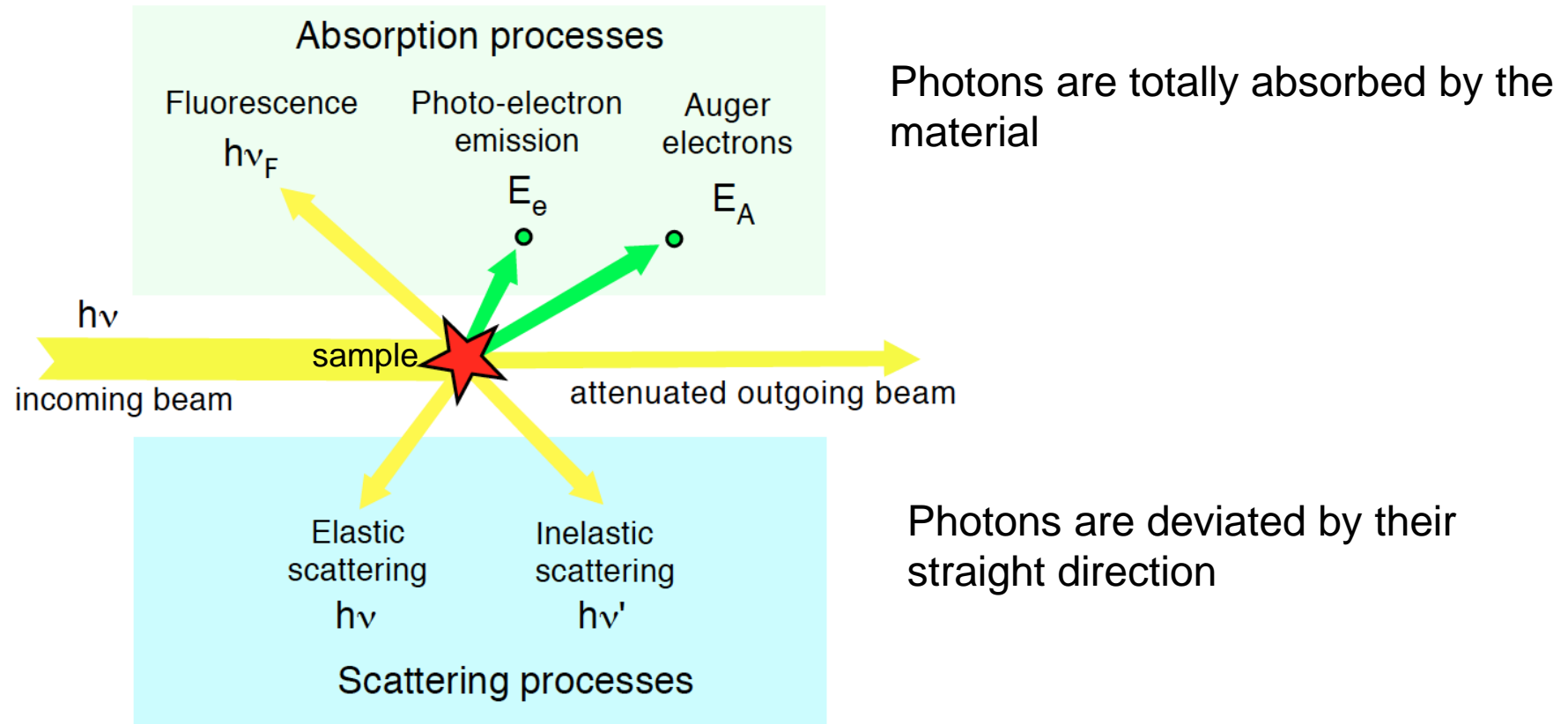


Neutrons:
Nuclear and magnetic interaction

X-rays:
Electromagnetic and core-hole interactions

Electrons:
Electrostatic interaction

X-RAY MATTER INTERACTION



Photon absorption/emission : Excitation with or without emission of electrons

Photon scattering :

Elastic coherent	=> Thomson
Inelastic incoherent	=> Compton
Resonant	=> elastic or inelastic

ELASTIC SCATTERING BY A FREE ELECTRON

- ◆ The incident electric field E_{in} forces the motion of the electron
- ◆ Electric Force $\mathbf{F}=q\mathbf{E}$ acting on an electron at rest
- ◆ Spherical wave re-radiation E_{rad}

Radiated spherical field E_{rad} at observer position R:

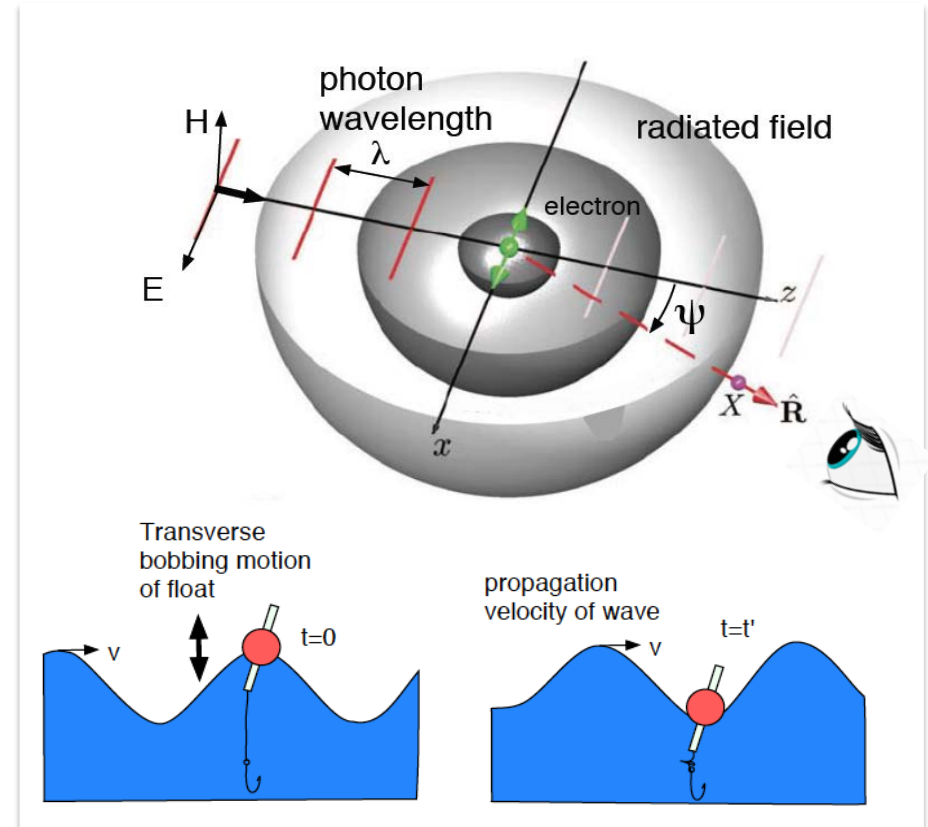
- proportional to the electron acceleration
- anti-phase with respect E_{in}
- decreases with $\cos(\psi)$

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

Thomson scattering length:

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

(Classical electron radius)

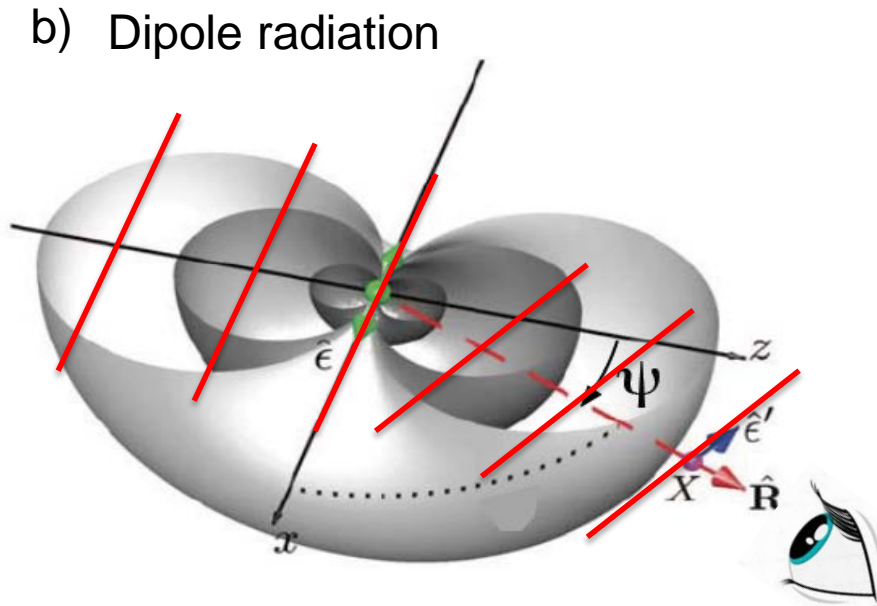
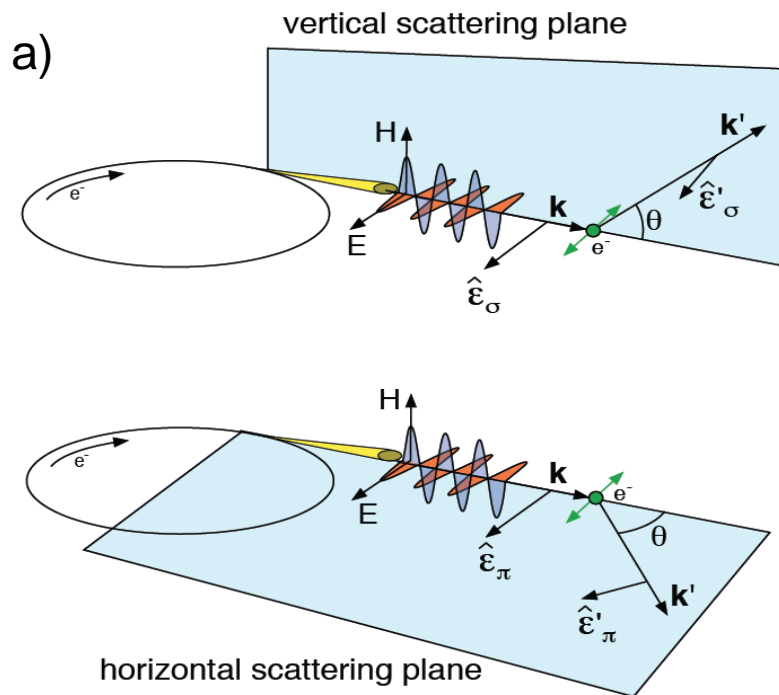


$$\frac{d\sigma}{d\Omega} = \frac{|E_{rad}|^2 R^2}{|E_{in}|^2} = r_0^2 |\hat{\epsilon} \cdot \hat{\epsilon}'|^2$$

POLARIZATION DEPENDENCE OF THOMSON SCATTERING

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

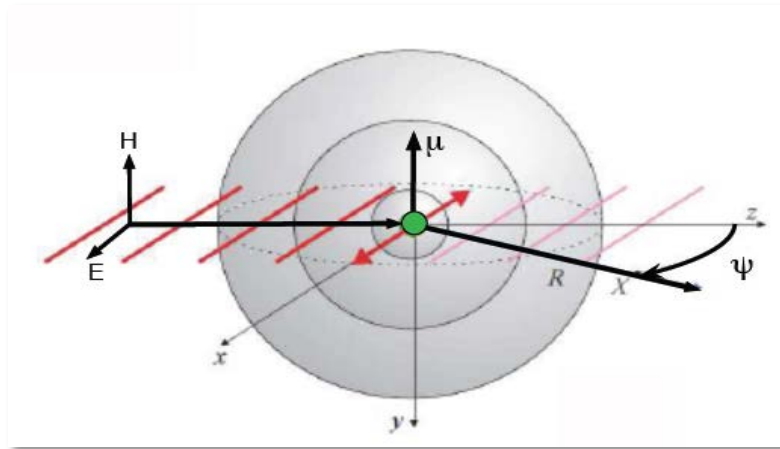
$$\left(\frac{d\sigma}{d\Omega}\right) = r_0^2 |\hat{\boldsymbol{\epsilon}} \cdot \hat{\boldsymbol{\epsilon}}'|^2 \quad P = |\hat{\boldsymbol{\epsilon}} \cdot \hat{\boldsymbol{\epsilon}}'|^2 = \begin{cases} 1 & \text{synchrotron: vertical scattering plane} \\ \cos^2 \psi & \text{synchrotron: horizontal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



MAGNETIC SCATTERING BY A FREE ELECTRON

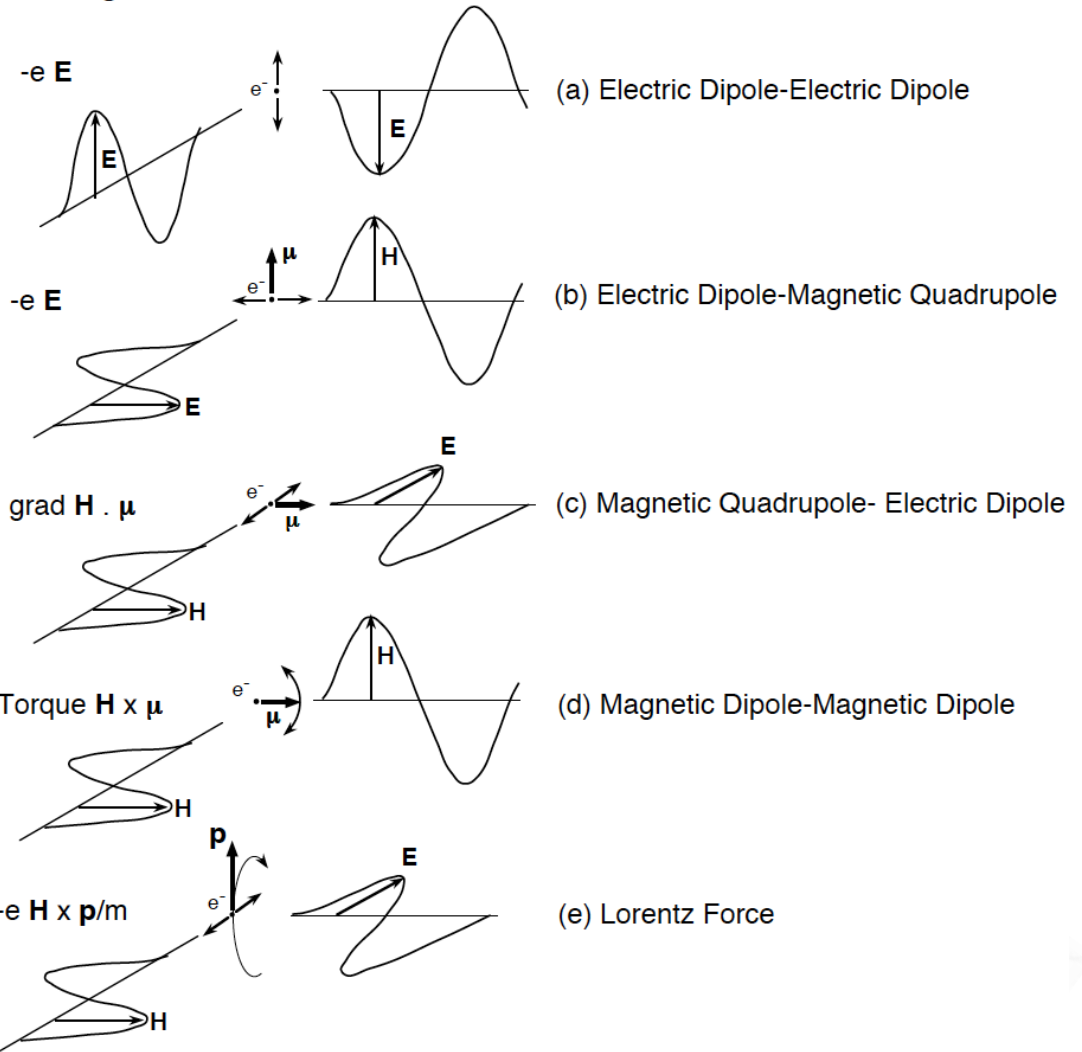
The magnetic scattering amplitudes are very weak because proportional to the relativistic factor E/mc^2

Both the \mathbf{H} magnetic and the electric \mathbf{E} field interact with the charge and magnetic moments of the electron



Driving Force

Re-radiation terms

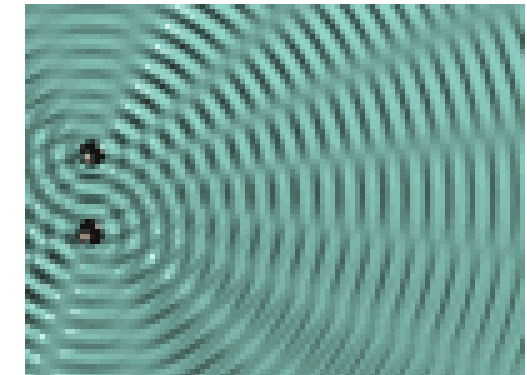
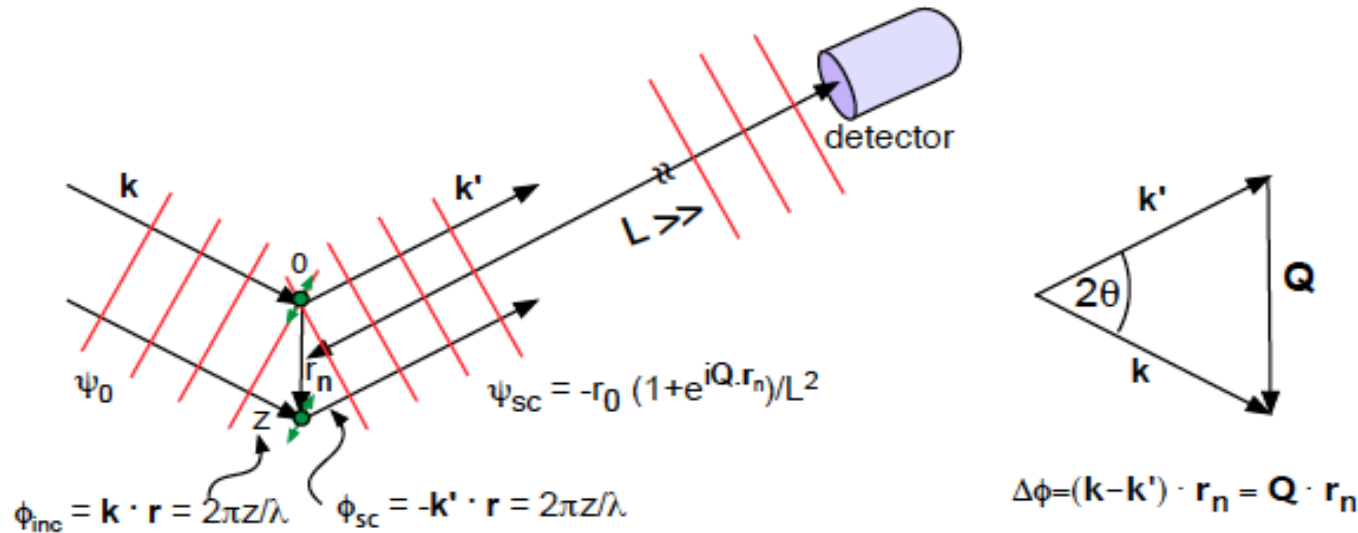


THOMSON SCATTERING BY TWO FREE ELECTRONS

- 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
- The phase difference between the two scattered X-rays is $\Delta\phi=(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r} = \mathbf{Q} \cdot \mathbf{r}$

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

Differential scattering cross section



Q = wavevector transfer or scattering vector

RANDOM DISTRIBUTION OF TWO ELECTRONS

The scattering intensity depends from the relative orientation of scattering vector \mathbf{Q} and the vector \mathbf{r}_n . (with neglect the polarization)

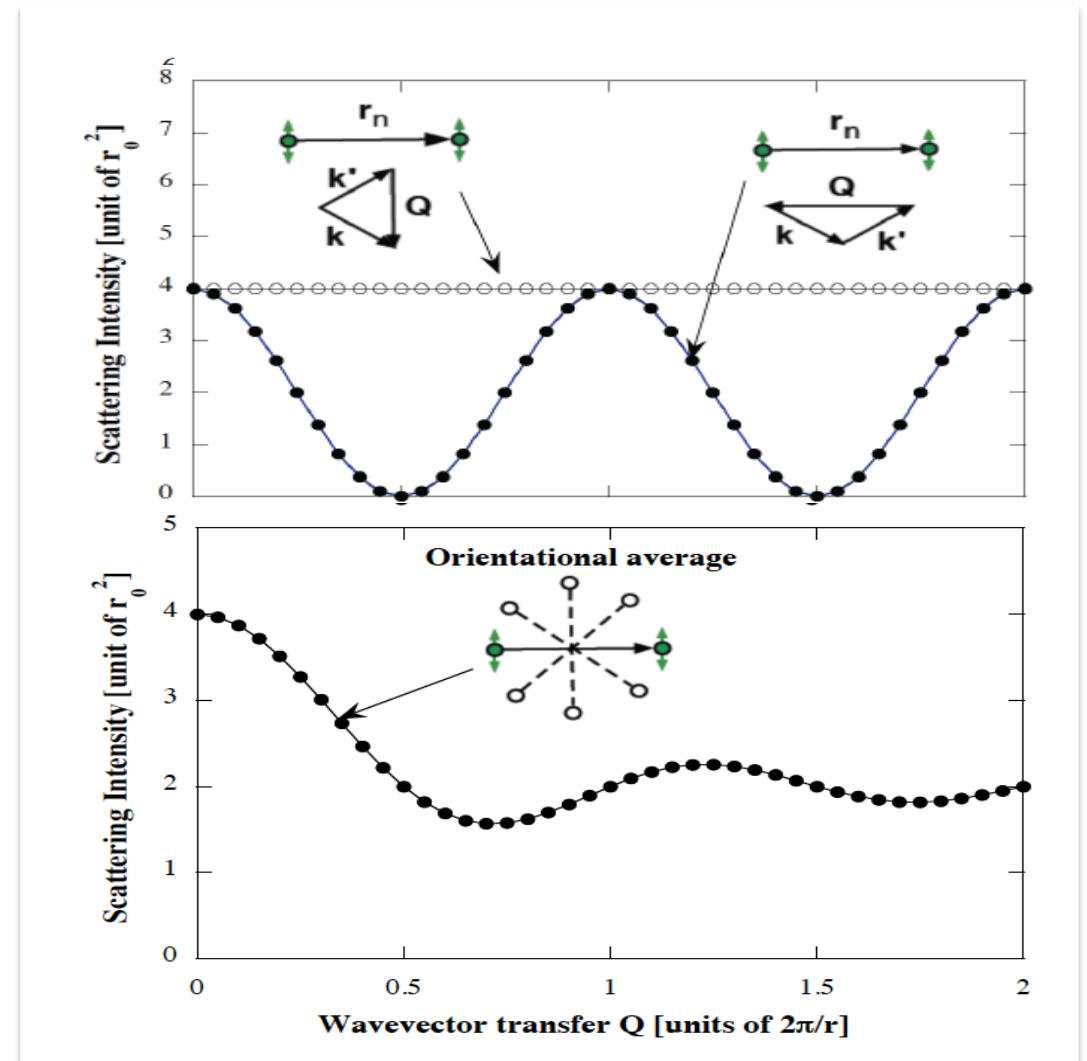
Scattering cross section (two electrons):

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

Scattering cross section (two electrons):
orientational average

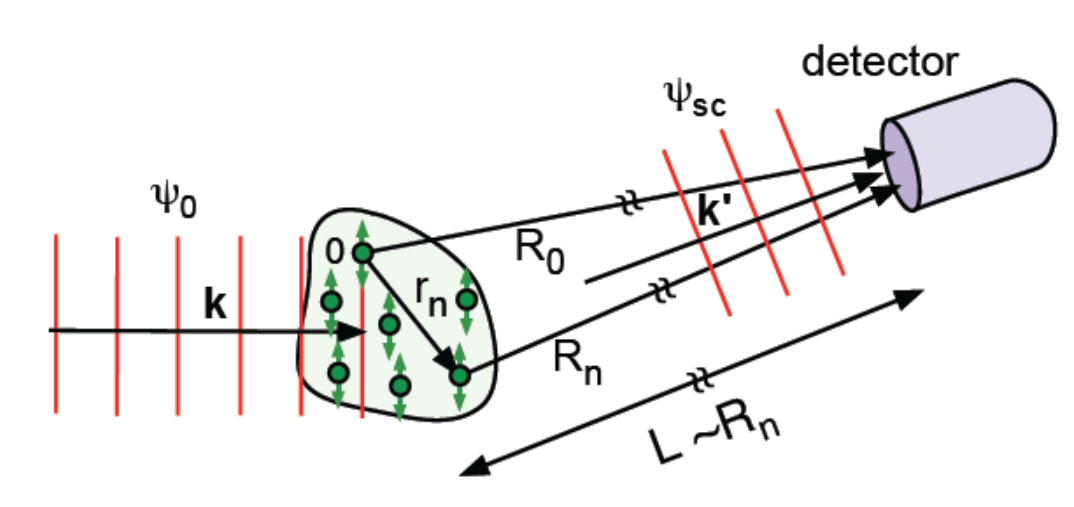
$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle_{\text{or.av.}} = 2r_0^2(1 + \langle e^{i\mathbf{Q} \cdot \mathbf{r}} \rangle_{\text{or.av.}})$$

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



THOMSON SCATTERING BY MANY ELECTRONS

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



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

Differential cross section for a charge spatial distribution

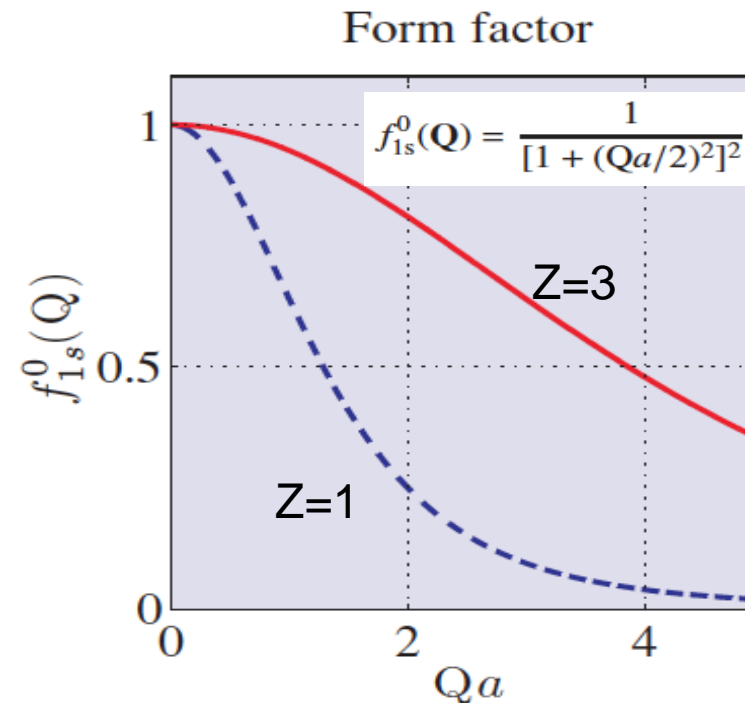
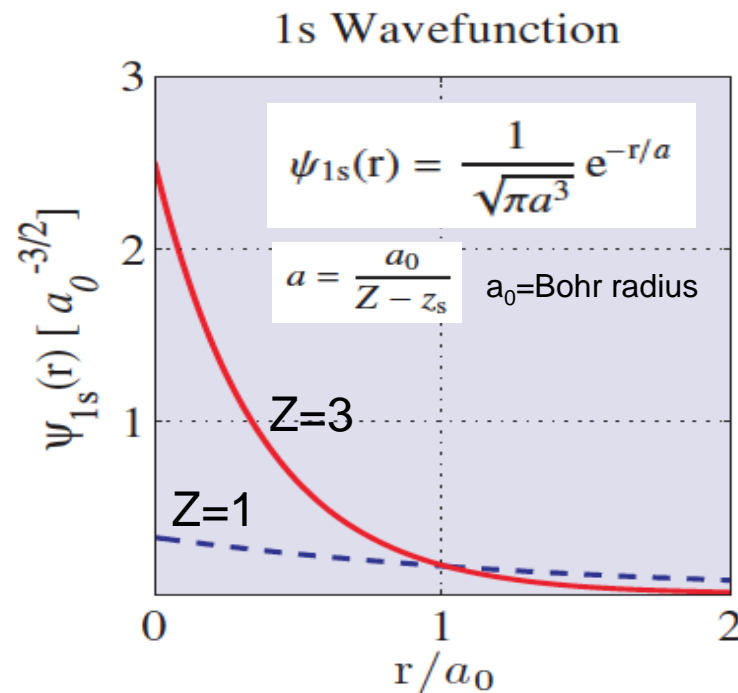
$$\frac{d\sigma}{d\Omega} = r_0^2 \left| \sum_n e^{i\mathbf{Q}\cdot\mathbf{r}_n} \right|^2$$

THOMSON SCATTERING BY ONE ATOM

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

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

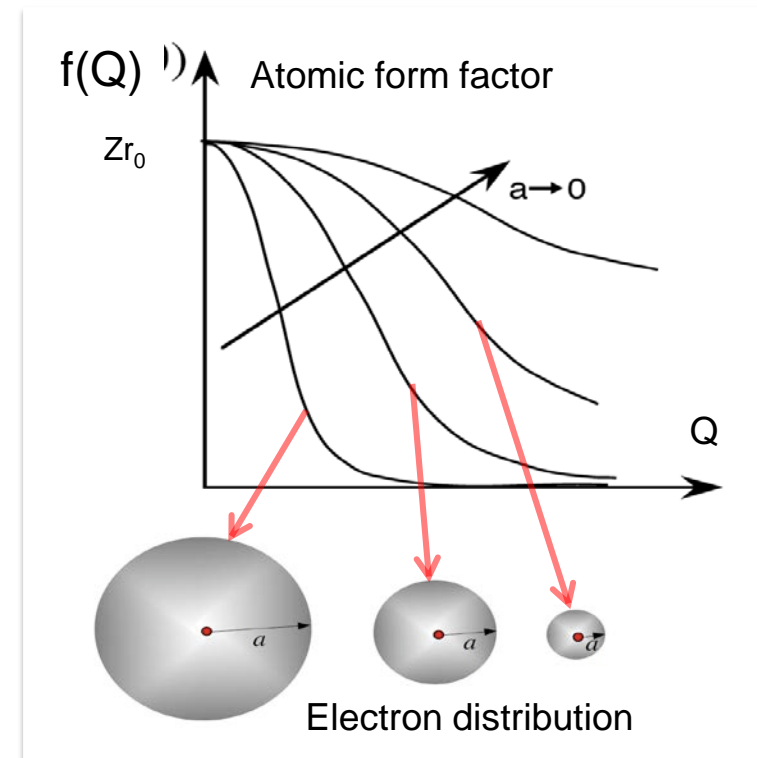
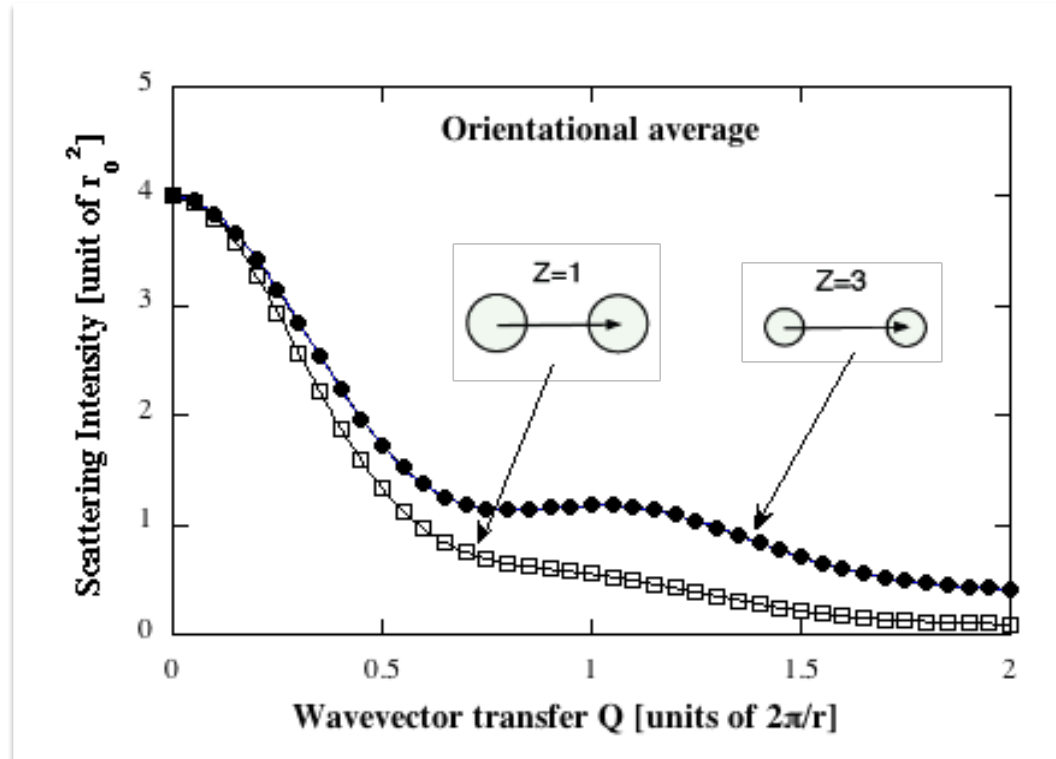
The Q dependence is due to the fact that the Thomson scattering is produced by all atomic electrons, which have a spatial extent of the same order of magnitude as the X-ray wavelength.



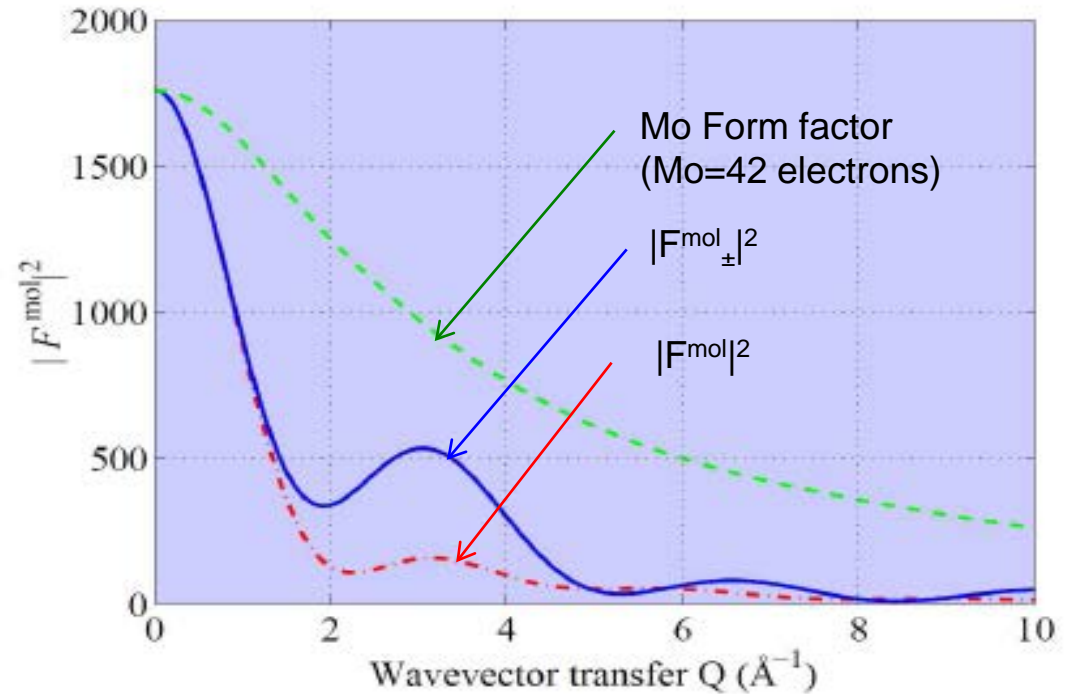
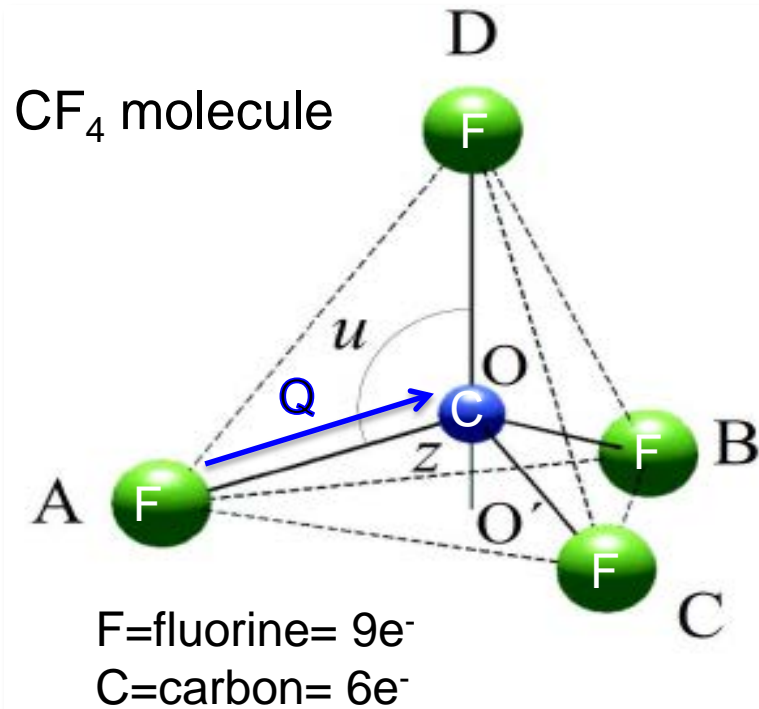
SCATTERING BY TWO ATOMS

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

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



SCATTERING FROM A MOLECULE



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

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

COMPTON SCATTERING (BY A FREE ELECTRON)

Inelastic collision between a photon and an electron at the rest in which part of the the photon energy is transferred to the electron (photon “red shift”)

This scattering is **incoherent** and contribute only to the background.

$$\lambda' = \lambda + \frac{h}{m_e c^2} (1 - \cos \psi) = \lambda + \lambda_c (1 - \cos \psi)$$

Maximum variation $\Delta\lambda=2\lambda_c$ when $\psi=180^\circ$

No variation when $\psi=0^\circ$

Compton scattering wavelength

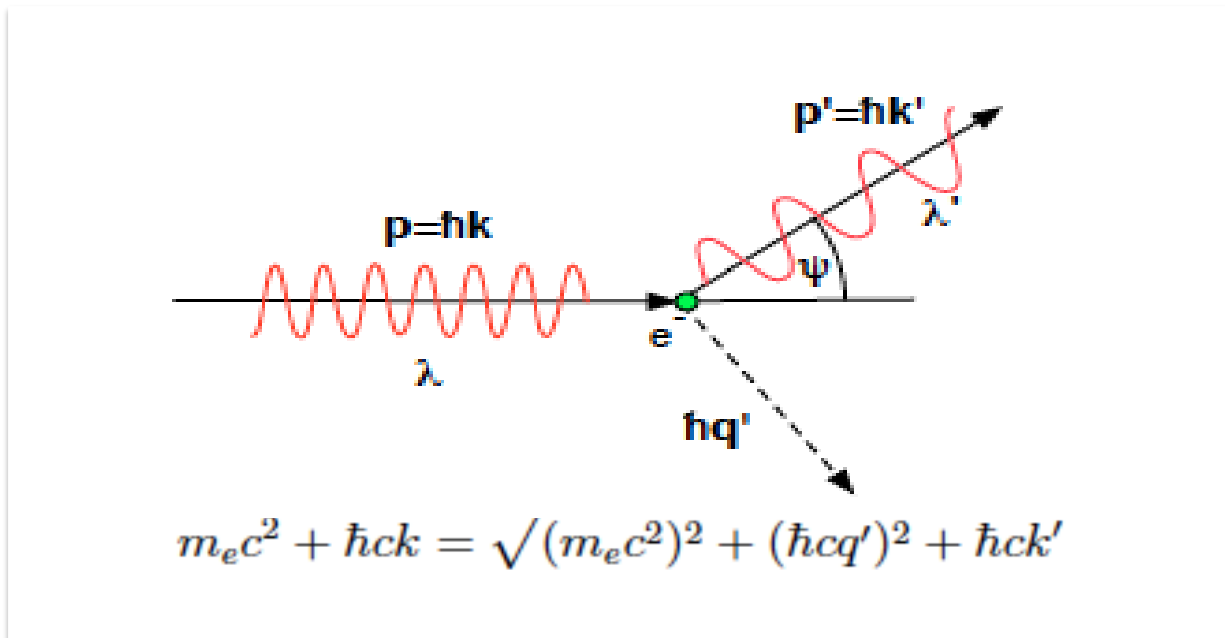
$$\lambda_c = \frac{h}{m_e c^2} = 0.0243 \text{ \AA}$$

Fine structure constant

$$\alpha = \frac{r_0}{(\lambda_c/2\pi)} = \frac{1}{137}$$

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

Maximum “red-shift” when $\psi=180$ deg.



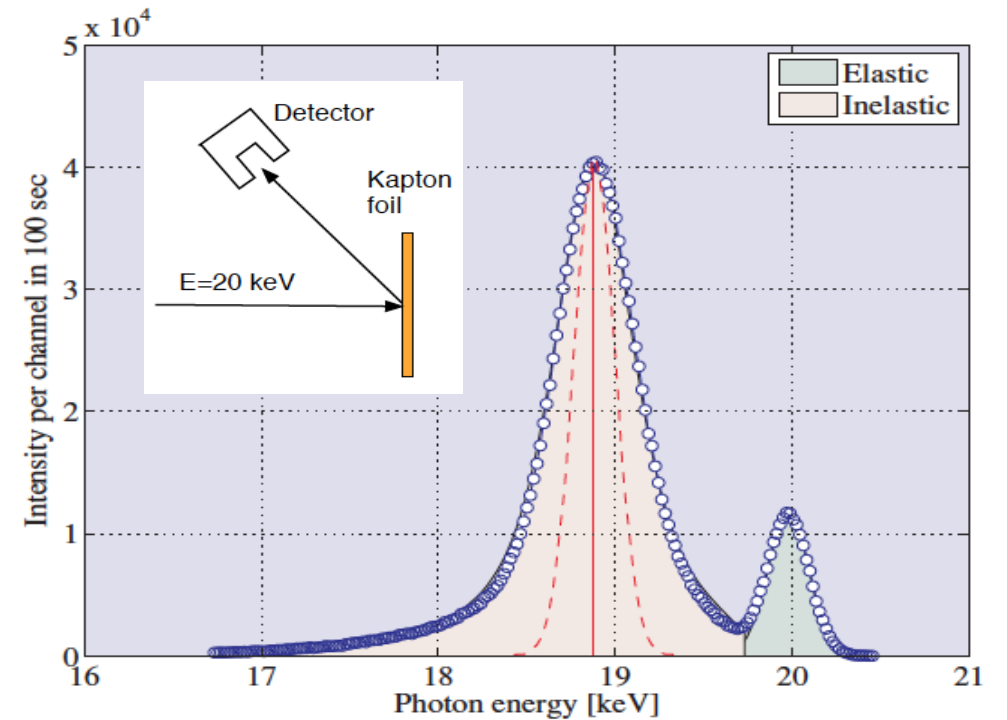
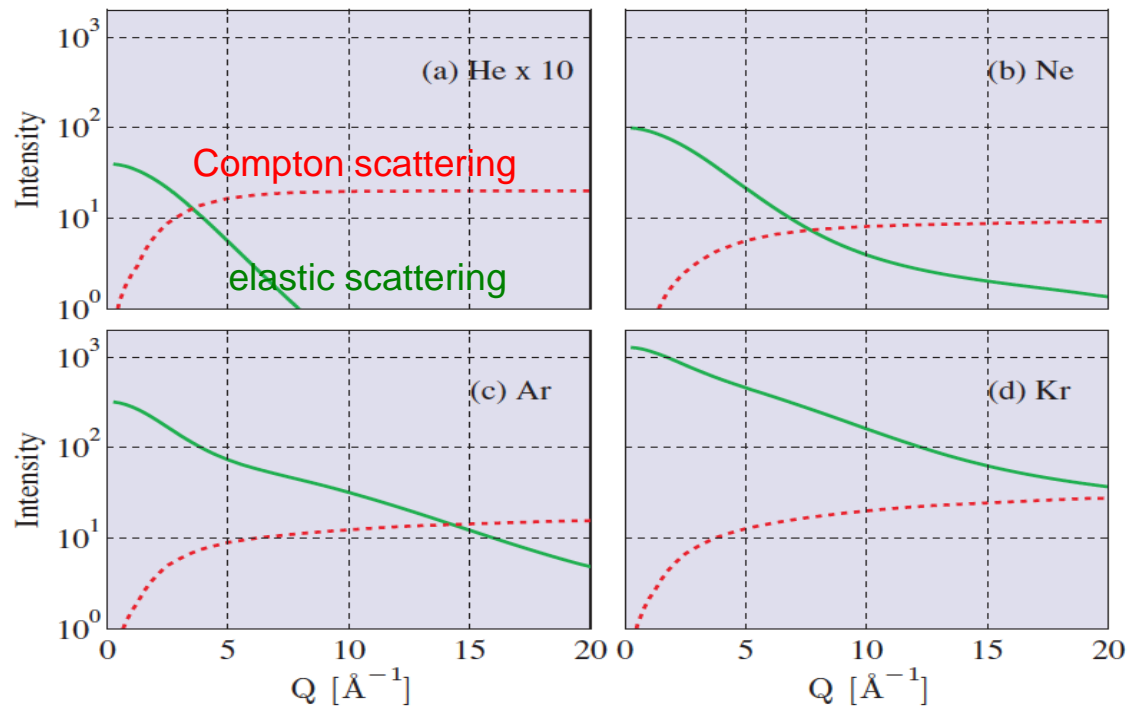
INCOHERENT INELASTIC COMPTON SCATTERING

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

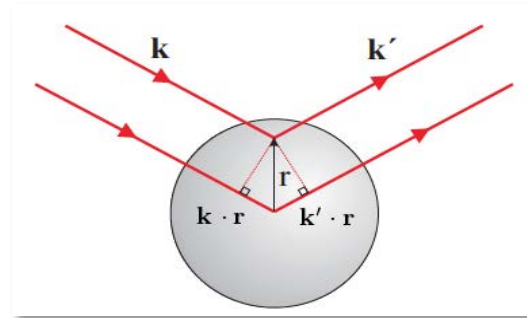


COHERENT ELASTIC SCATTERING(THOMSON)

Scattering processes conserve the number of photons

If the photon energy is conserved, the scattering is elastic. If not. It is inelastic

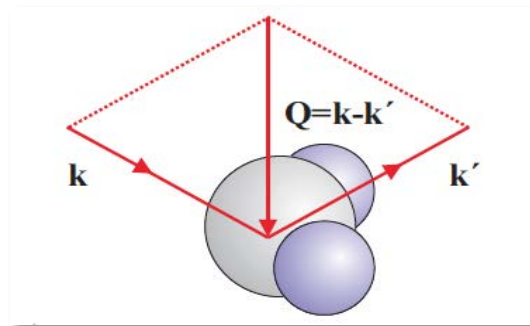
one atom



Atomic form factor

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

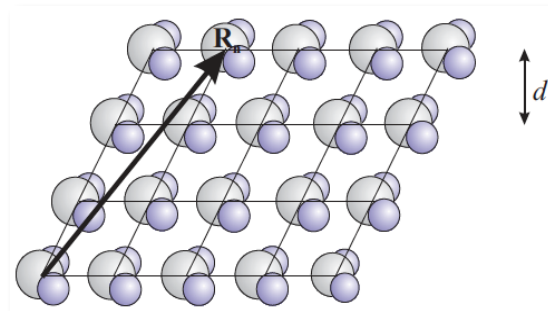
a molecule



Molecule structure factors

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

a crystal



Crystal structure factors

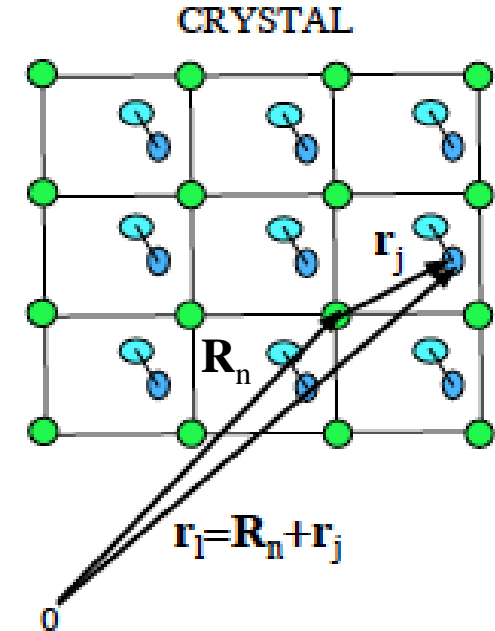
$$F^{\text{crystal}}(\mathbf{Q}) = \underbrace{\sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}}_{\text{Unit cell structure factor}} \underbrace{\sum_n e^{i\mathbf{Q}\cdot\mathbf{R}_n}}_{\text{Lattice sum}}$$

CRYSTAL STRUCTURE FACTOR

The Fourier transform of the crystal (the crystal structure factor) is equal to the product of the FT of lattice and the basis

$$\begin{aligned}
 F^{crystal}(\mathbf{Q}) &= -r_0 \sum_{\mathbf{R}_n + \mathbf{r}_j}^{all\ atoms} f_j(\mathbf{Q}) e^{i\mathbf{Q} \cdot (\mathbf{R}_n + \mathbf{r}_j)} \\
 &= -r_0 \sum_n^{lattice} e^{i\mathbf{Q} \cdot \mathbf{R}_n} \sum_j^{unit\ cell} f_j(\mathbf{Q}) e^{i\mathbf{Q} \cdot \mathbf{r}_j}
 \end{aligned}$$

FT Lattice
FT Basis



$$S_N(\mathbf{Q}) = \sum_n^{lattice} e^{i\mathbf{Q} \cdot \mathbf{R}_n}$$

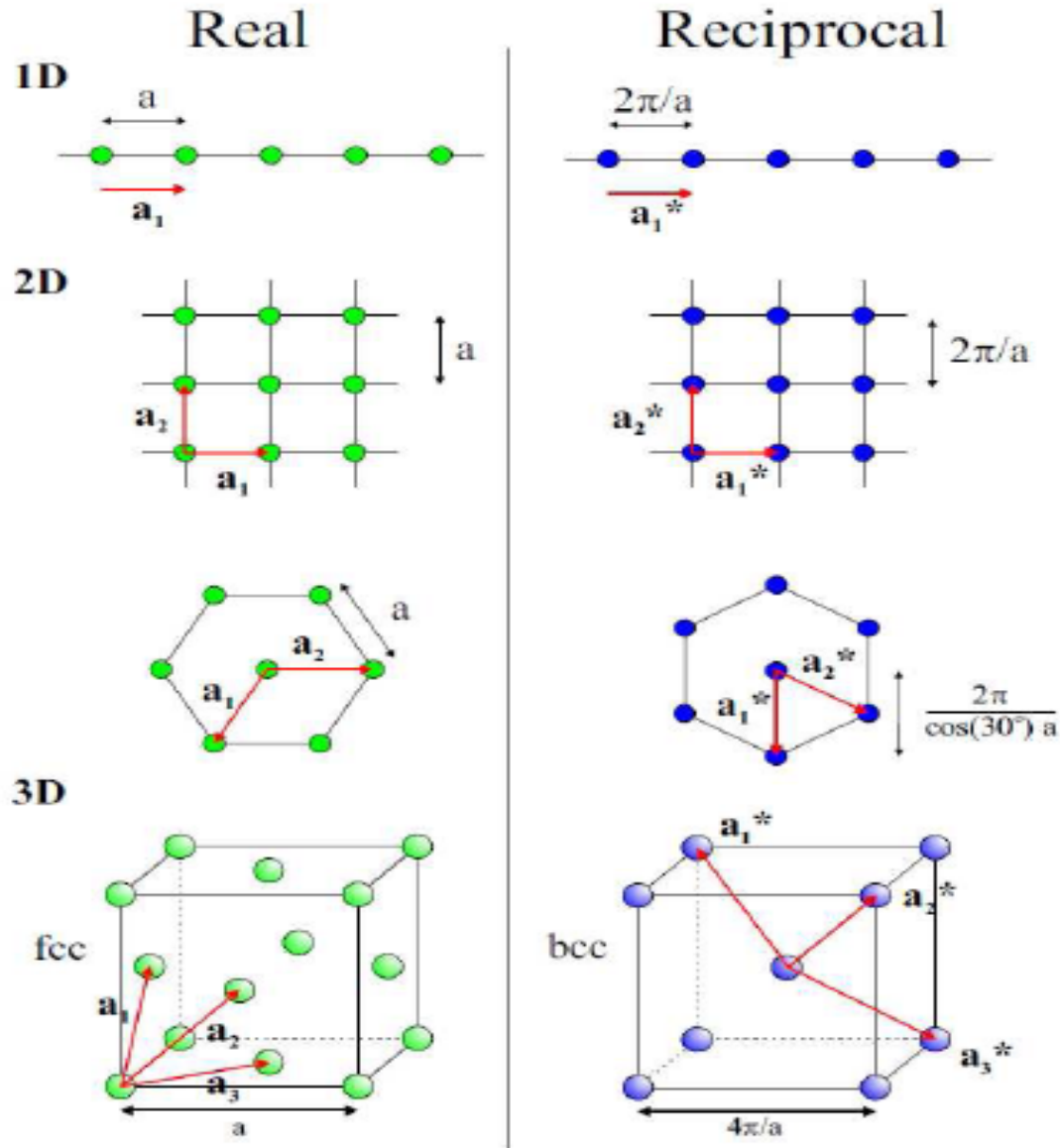
The lattice sum is non vanishing only when:

$$\mathbf{Q} \cdot \mathbf{R}_n = 2\pi \times \text{integer}$$

$$\mathbf{G}_{hkl} \cdot \mathbf{R}_n = 2\pi \times \text{integer} = 2\pi(hn_1 + kn_2 + ln_3)$$

Laue conditions

EXAMPLE OF RECIPROCAL SPACES



Example: fcc lattice

$$\mathbf{a}_1 = \frac{a}{2}(\hat{y} + \hat{z})$$

$$\mathbf{a}_2 = \frac{a}{2}(\hat{z} + \hat{x})$$

$$\mathbf{a}_3 = \frac{a}{2}(\hat{x} + \hat{y})$$

$$\mathbf{a}_1^* = \frac{4\pi}{a} \left(\frac{\hat{y}}{2} + \frac{\hat{z}}{2} - \frac{\hat{x}}{2} \right)$$

$$\mathbf{a}_2^* = \frac{4\pi}{a} \left(\frac{\hat{z}}{2} + \frac{\hat{x}}{2} - \frac{\hat{y}}{2} \right)$$

$$\mathbf{a}_3^* = \frac{4\pi}{a} \left(\frac{\hat{x}}{2} + \frac{\hat{y}}{2} - \frac{\hat{z}}{2} \right)$$

EQUIVALENCE BRAGG-LAUE

Bragg's law:

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

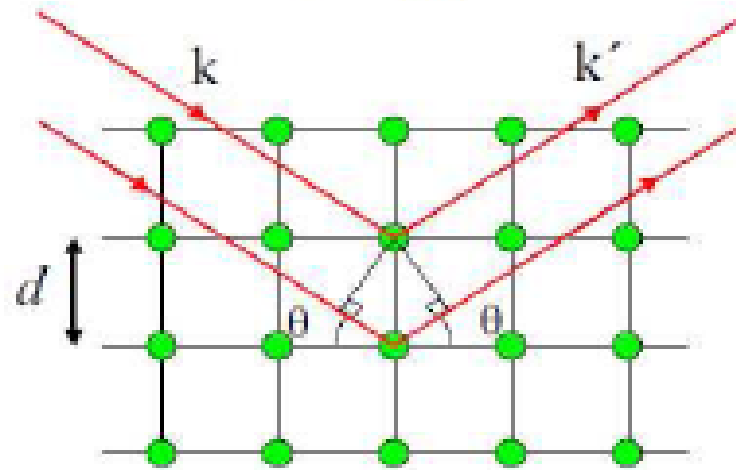
Laue's condition

$$\mathbf{k}' - \mathbf{k} = \mathbf{Q} = 2\pi \mathbf{G}_{hkl}$$

$$|\mathbf{G}_{hkl}| = 2\pi / d_{hkl}$$

Bragg

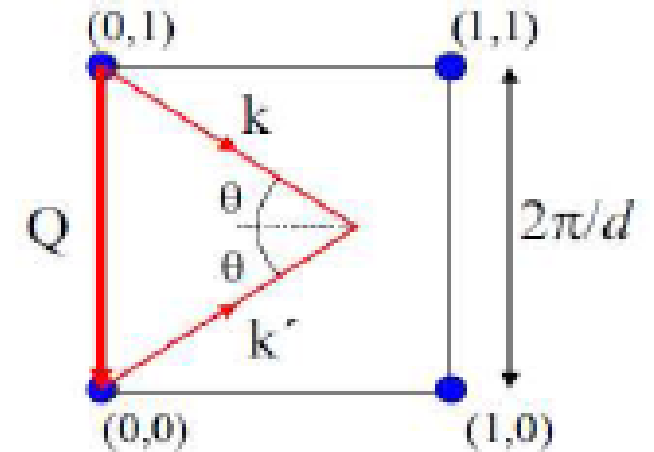
$$\lambda = 2d \sin \theta$$



Real

Laue

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



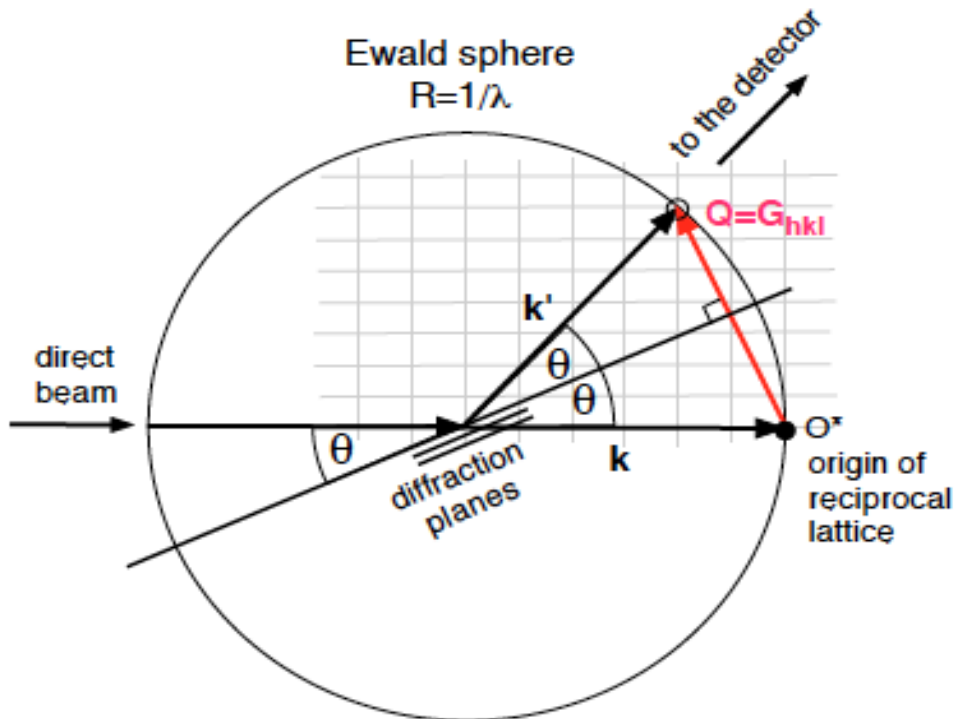
Reciprocal

$$\left(\frac{d\sigma}{d\Omega} \right)_{\text{Bragg}} = N \frac{(2\pi)^3}{v_0} r_0^2 \sum_{hkl} \delta(\mathbf{Q} - \mathbf{G}_{hkl}) |F(hkl)|^2$$

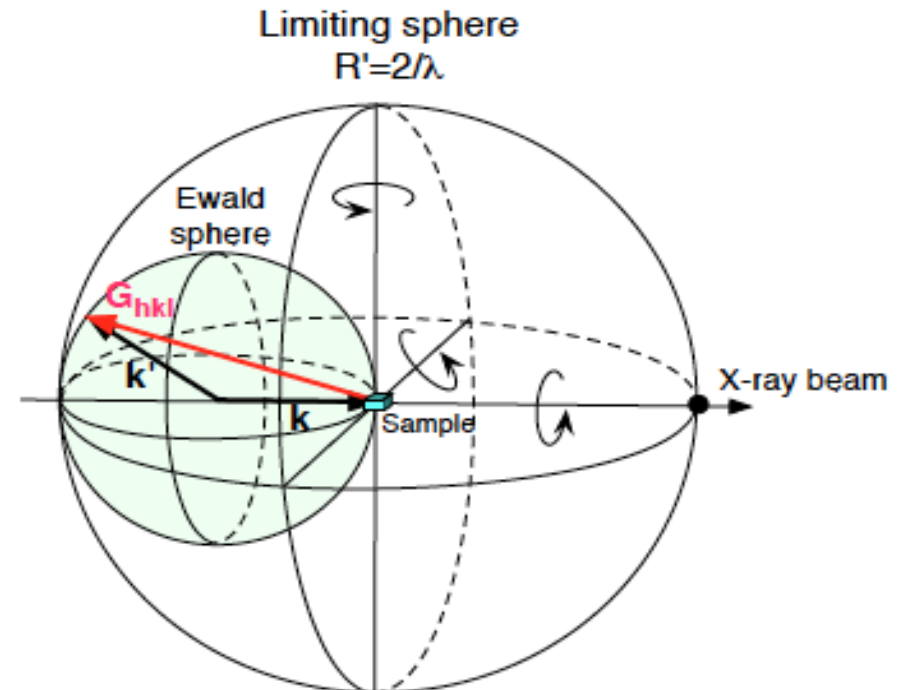
Differential cross section for the Bragg diffraction in crystals

EWALD SPHERE

Geometric construction that allows one to visualize the Bragg' law during the elastic diffraction experiment



Only all the reciprocal lattice points G_{hkl} intercepting the Ewald sphere fulfill the Bragg conditions



All the G_{hkl} contained in limiting sphere could be reached by rotating the sample about the goniometer axis

POWDER DIFFRACTION

Size and symmetry of the unit cell

Debye-Scherrer cone

$$2\pi |\mathbf{G}|_{hkl} \sin\left(\frac{\pi}{2} - \theta\right) = 2\pi |\mathbf{G}|_{hkl} \cos \theta$$

Detector aperture δ

$$\delta k / (2k \sin 2\theta)$$

$$I(hkl)_{\text{Powder}} = |F_{hkl}|^2 m_{hkl} \cos \theta \frac{1}{\sin 2\theta} \frac{1}{\sin 2\theta} P(\cos 2\theta_{hkl})$$

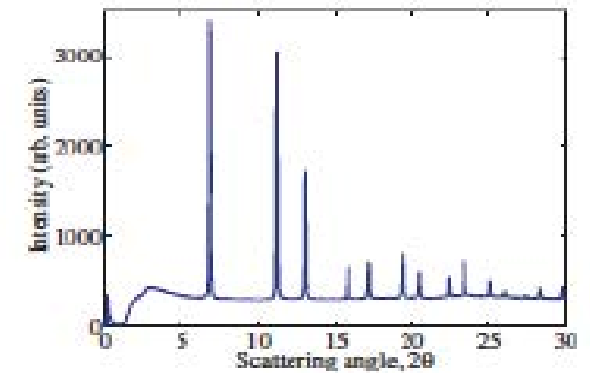
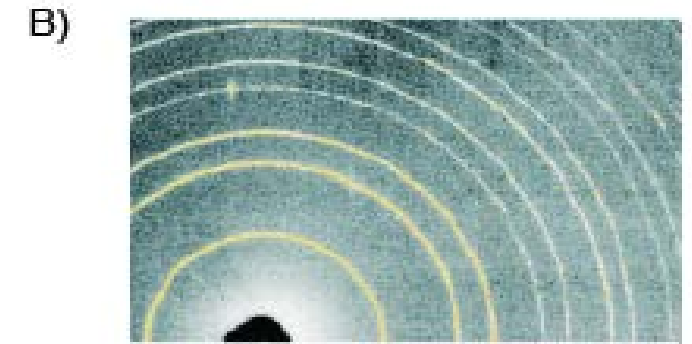
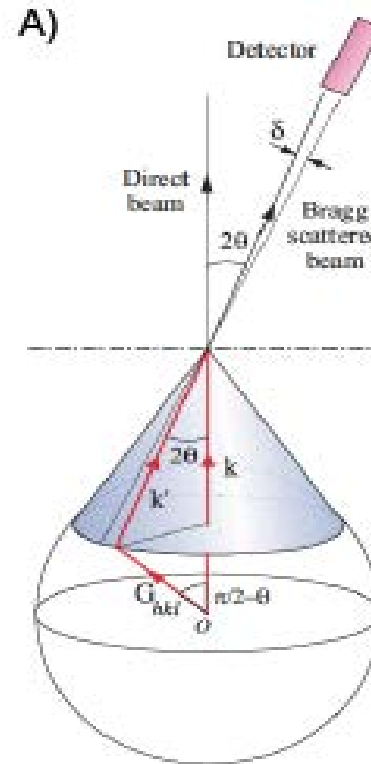
Multiplicity m_{hkl}

$m_{hkl} \cos \theta$

Lorentz factor

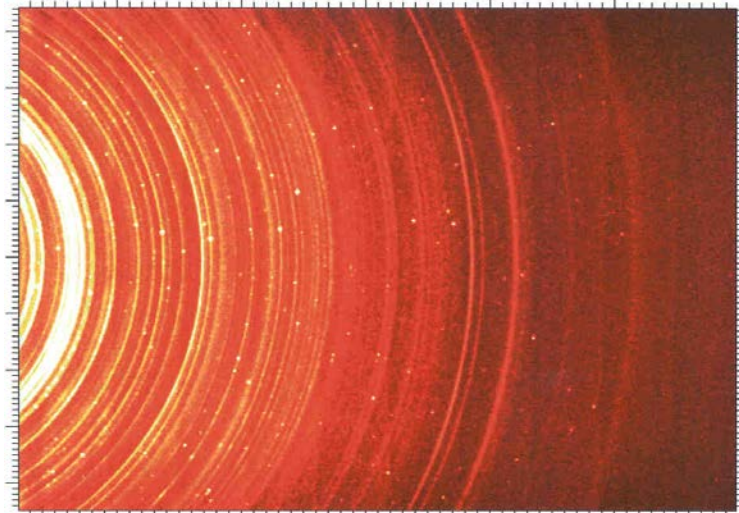
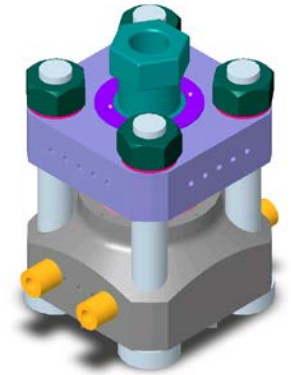
$\frac{1}{\sin 2\theta}$

Polarization factor

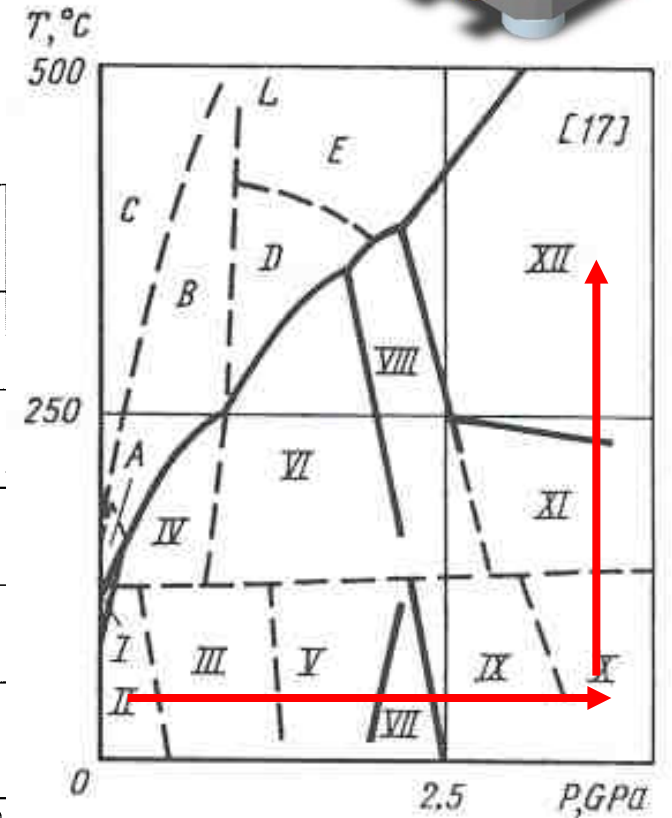
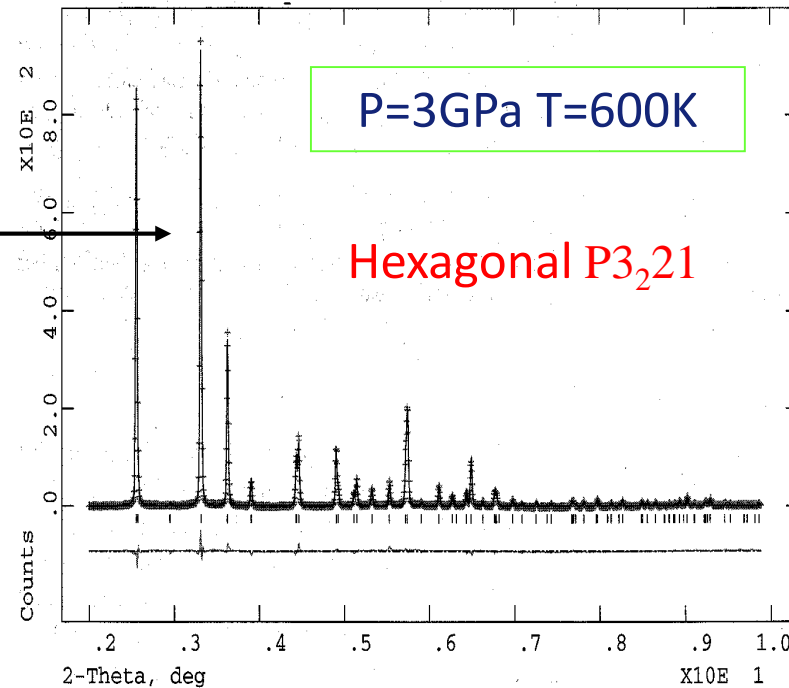
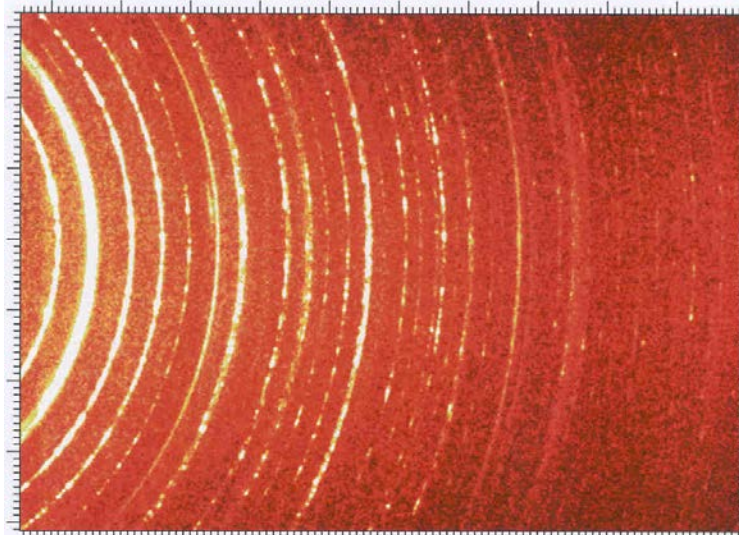


EXAMPLE : HIGH PRESSURE SYNTHESIS OF SULFUR

- Pressure up to 17 GPa on 2 mm³ sample volume
- Resistive heating up to 2000 K



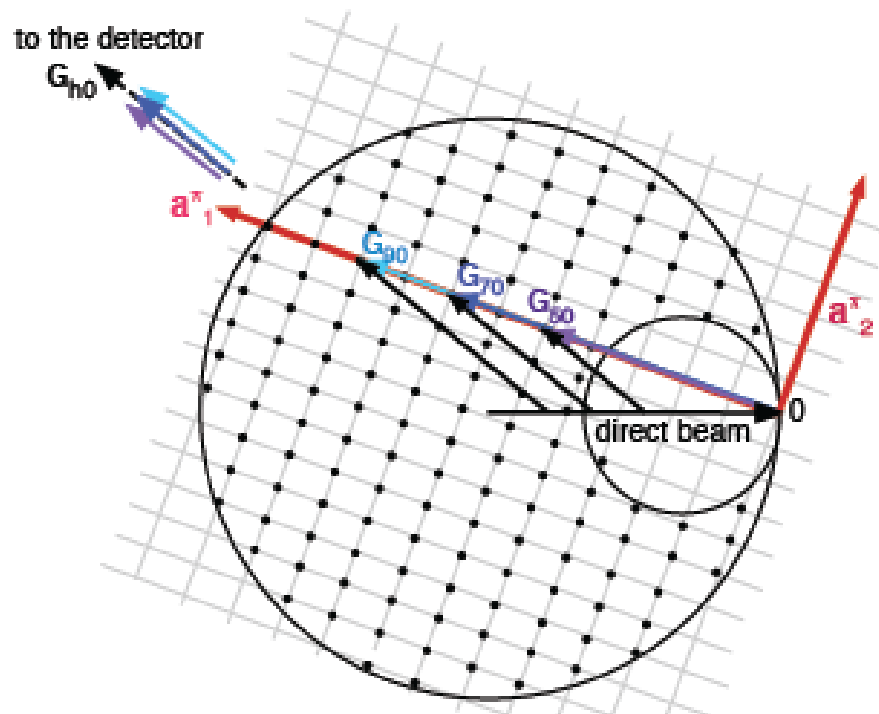
At RT-RP, Orthorhombic Fddd based on S₈ rings (molecular units)



WHITE BEAM LAUE PATTERN

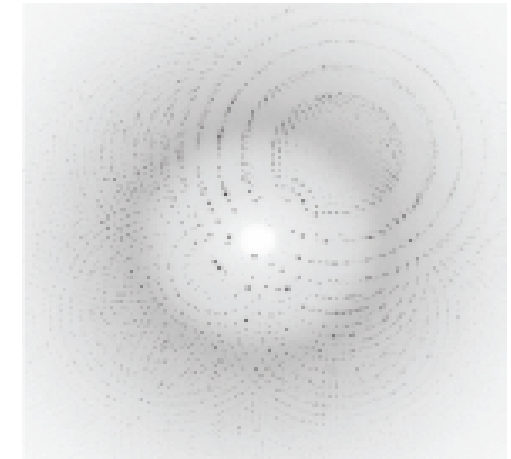
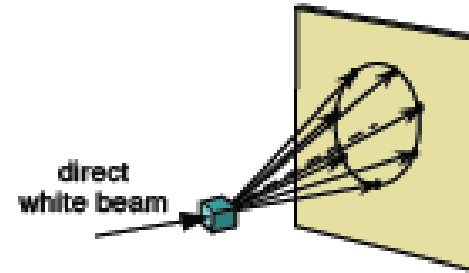
Polychromatic beam technique used in protein crystallography or in more complex structures.
Data collection of a large number of reflections

a)

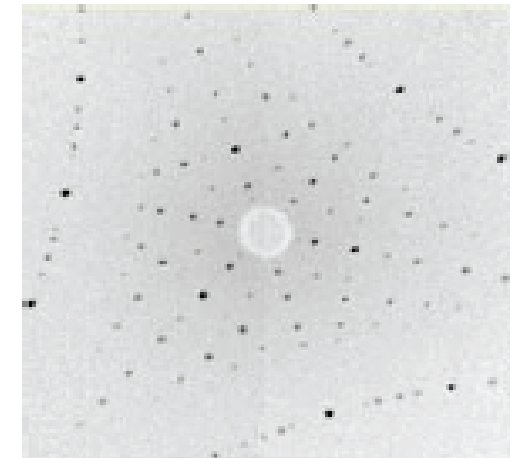
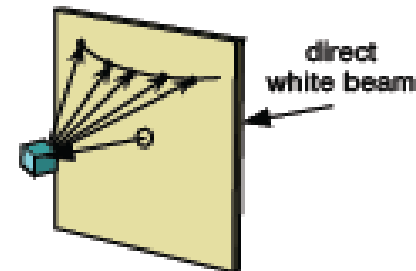


All the lattice points contained in the grey area contribute to the Bragg diffraction

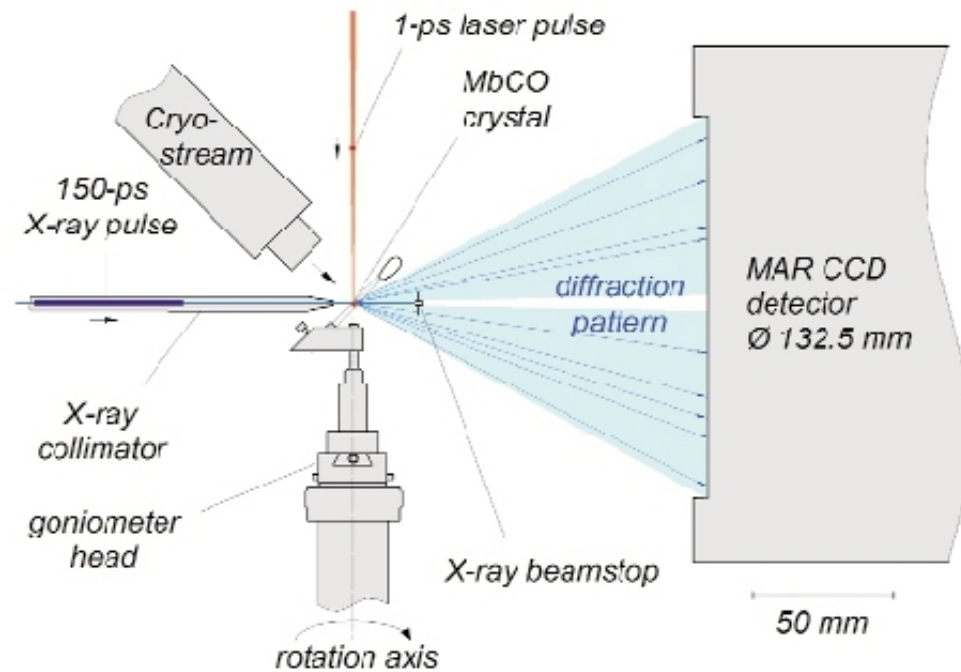
b) Transmission Laue



c) Back-scattering Laue

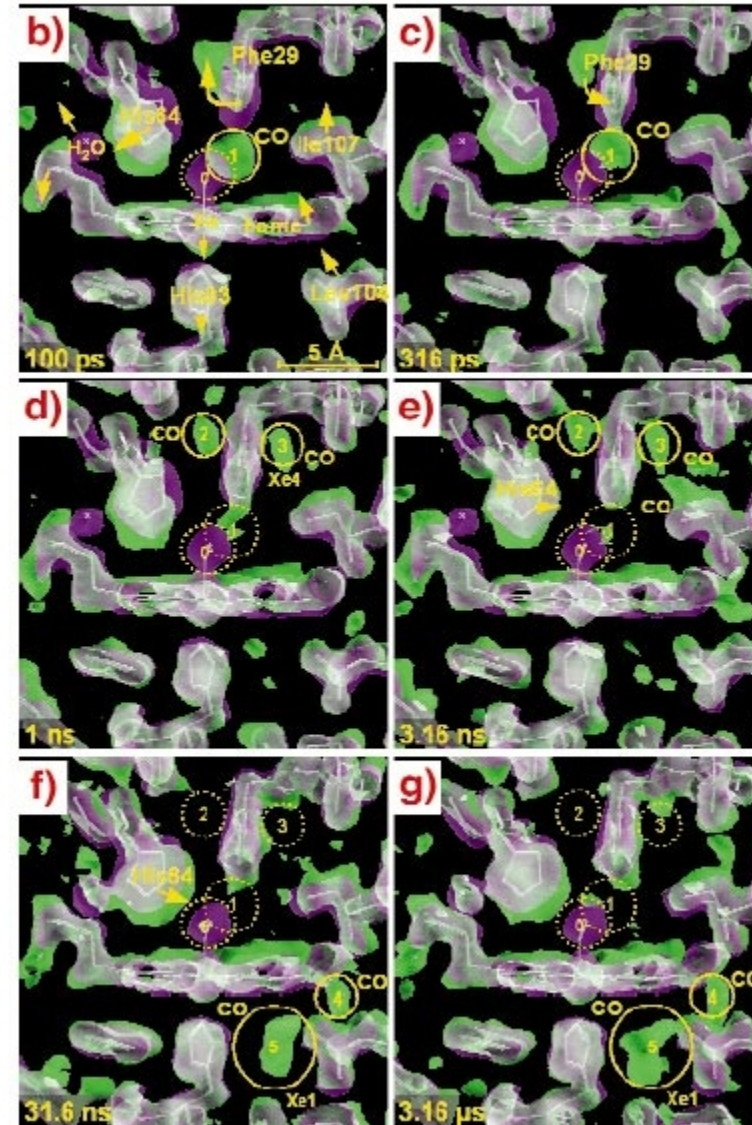


Time-resolved MX using the Laue technique (White/Pink beam)

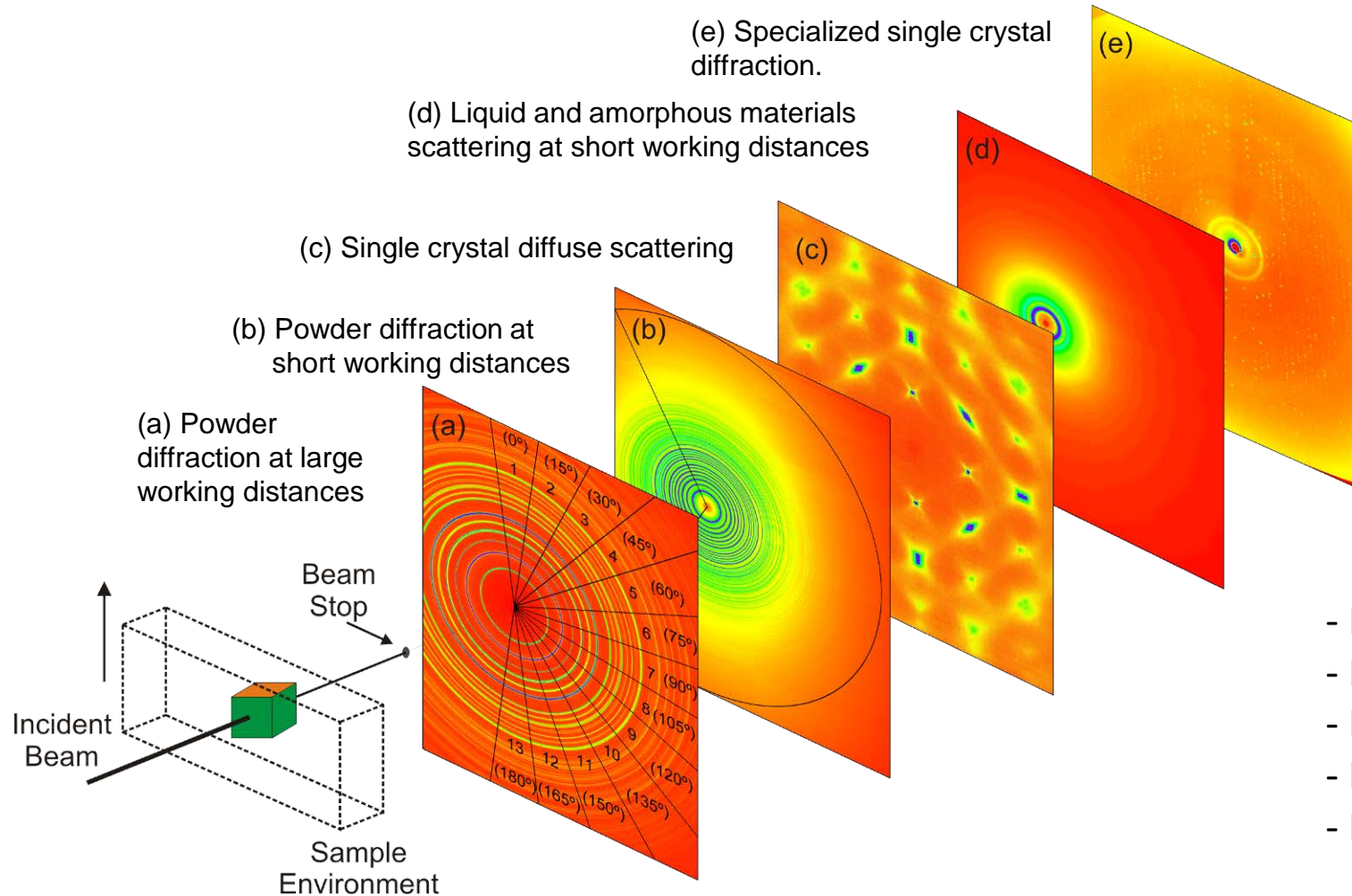


Structure of MbCO at different time delays after photolysis. The bound CO dissociates, eventually becoming trapped in sites 4 and 5, where it remains out to the microsecond time scale.

F. Schotte *et al.*, (2003), *Science*, 300, 1944-1947.



- Multi-length scale problems

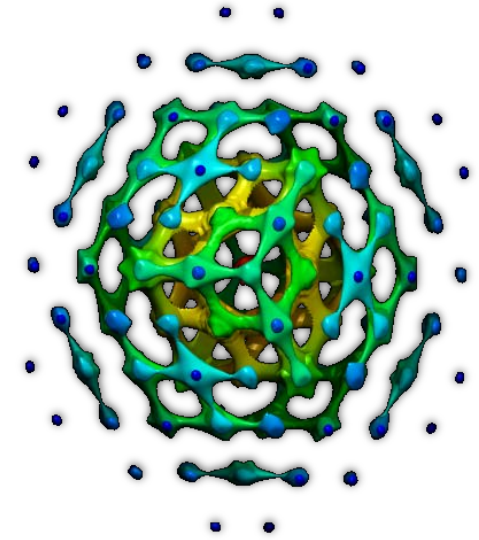


- Large input surface (>150 mm diameter)
- High spatial resolution (50 to 100 μm)
- High dynamic range (14 bits or more)
- High sensitivity (quantum efficiency)
- Fast read-out (a few seconds or less)

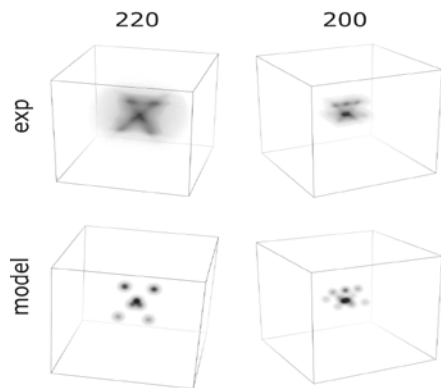
State-of-the-art methods for diffuse scattering/diffraction studies of crystalline materials

- Direct space real structure of systems with correlated disorder
- Time-resolved diffuse scattering studies of phase transitions
- Electron-phonon coupling in strongly correlated electron system
- Shape determination of Fermi surface in metallic systems
- Vibrational properties of nano-modulated and low-dimensional systems

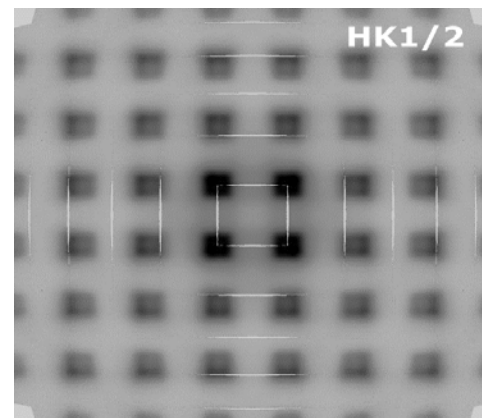
➤ Absorption



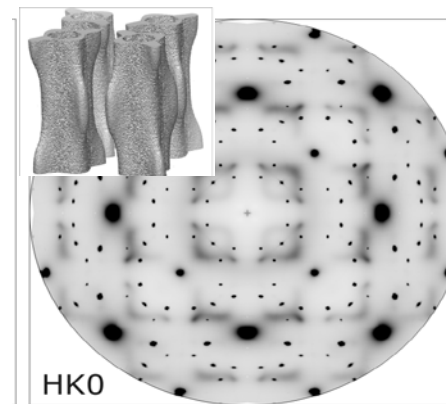
Multiple phase crystal



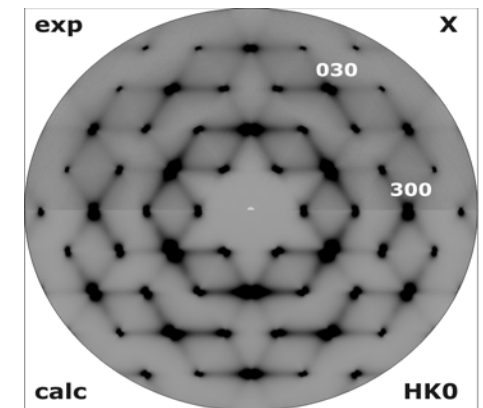
Static disorder



Structured diffuse scattering



Thermal diffuse



Inelastic X-ray scattering

LATTICE VIBRATIONS

Vibrations around equilibrium position

$\mathbf{u}_n(t)$ Instantaneous displacement
Around the equilibrium position

$\langle \mathbf{u}_n \rangle = 0$ Temporal (thermal) average

Origin: - Thermal vibration
- Zero point fluctuations

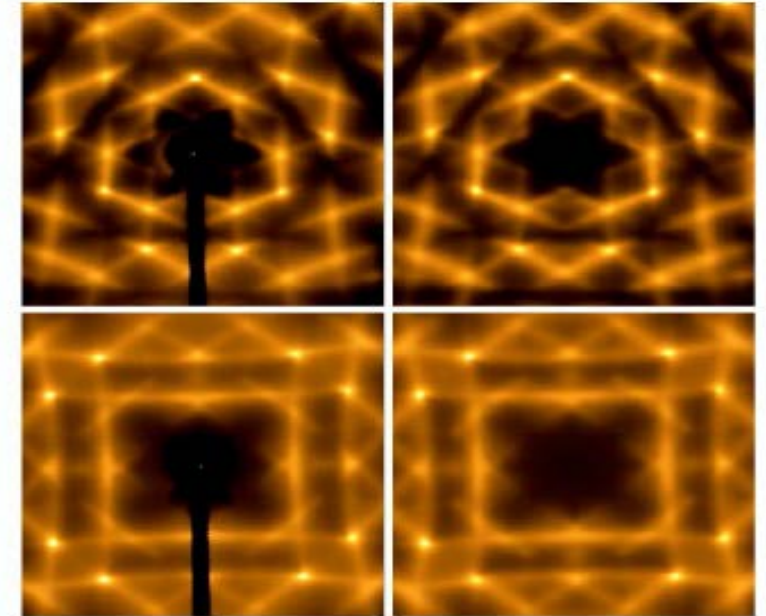
Instantaneous structure factor:

$$F^{crystal}(\mathbf{Q}, t) = -r_0 \sum_n^{all\ atoms} f_n(\mathbf{Q}) e^{i\mathbf{Q} \cdot (\mathbf{R}_n + \mathbf{u}_n(t))}$$

Scattering intensity proportional to the thermal average

$$\begin{aligned} I(\mathbf{Q}) &= \langle F(\mathbf{Q}, t) F^*(\mathbf{Q}, t) \rangle \\ &= r_0^2 \sum_n \sum_m f_n(\mathbf{Q}) f_m^*(\mathbf{Q}) e^{i\mathbf{Q} \cdot (\mathbf{R}_n - \mathbf{R}_m)} \langle e^{i\mathbf{Q} \cdot (\mathbf{u}_n - \mathbf{u}_m)} \rangle \end{aligned}$$

Thermal diffuse scattering:



INELASTIC STRUCTURE FACTOR

Scattering intensity for the lattice vibrations

$$\begin{aligned}
 & \text{elastic part} \\
 I(\mathbf{Q}) &= r_0^2 \sum_n \sum_m f(\mathbf{Q}) f^*(\mathbf{Q}) e^{-2W} e^{i\mathbf{Q} \cdot \mathbf{R}_n} e^{-i\mathbf{Q} \cdot \mathbf{R}_m} \\
 & \text{Thermal diffuse scattering} \\
 & + r_0^2 \sum_n \sum_m f(\mathbf{Q}) f^*(\mathbf{Q}) e^{-2W} e^{i\mathbf{Q} \cdot \mathbf{R}_n} e^{-i\mathbf{Q} \cdot \mathbf{R}_m} \left[e^{Q^2 \langle u_{Qn} u_{Qm} \rangle} - 1 \right]
 \end{aligned}$$

Debye-Waller factor

- Independent from the inter-atom interactions
- Depends from Q^2
- Decreases the Bragg intensities

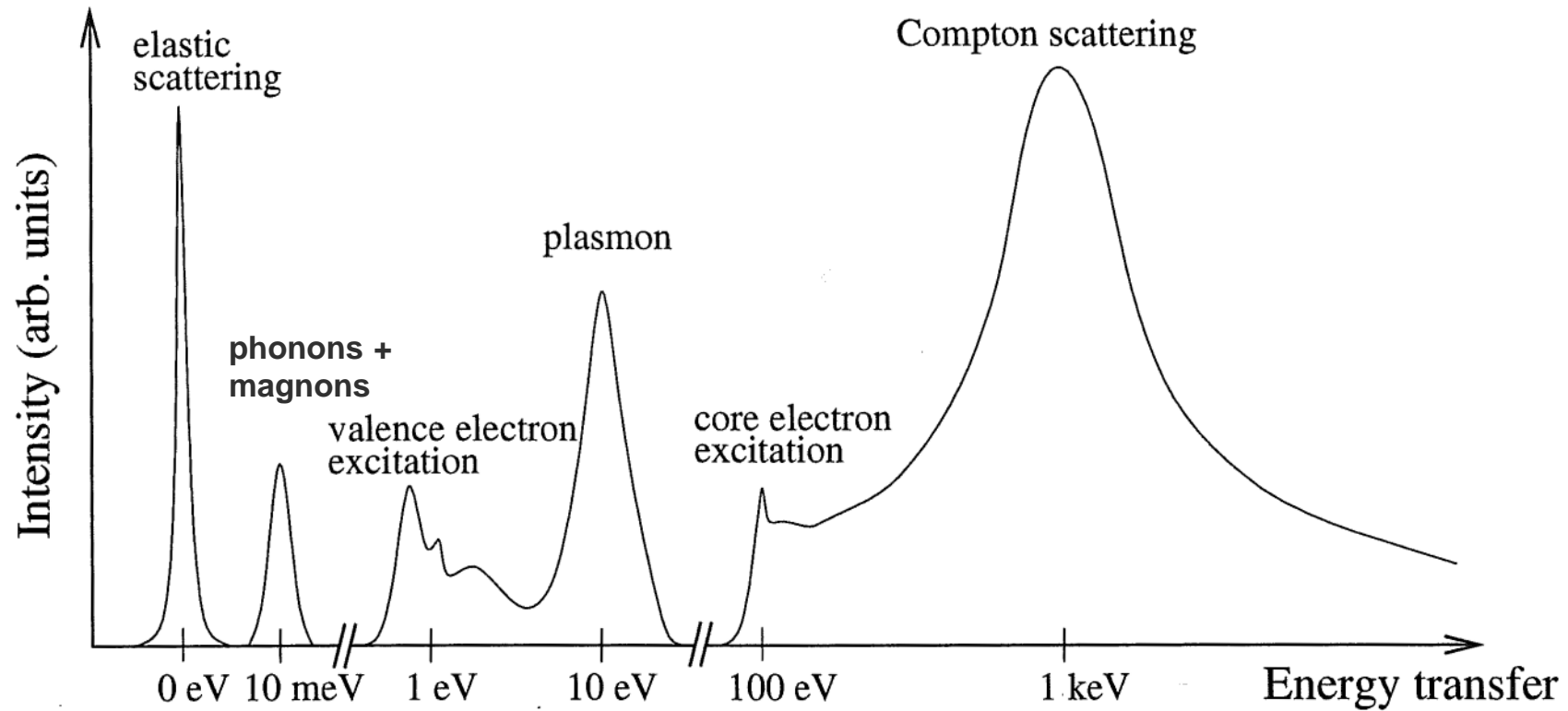
$$\begin{aligned}
 W_j &= \frac{1}{2} Q^2 \langle u_{Qj}^2 \rangle = \frac{1}{2} (2k \sin \theta)^2 \langle u_{Qj}^2 \rangle \\
 &= \frac{1}{2} \left(\frac{4\pi}{\lambda} \right)^2 \sin^2 \theta \langle u_{Qj}^2 \rangle = B_T^j \left(\frac{\sin \theta}{\lambda} \right)
 \end{aligned}$$

For isotropic vibrations

$$B_{T, \text{isotropic}} = \frac{8\pi^2}{3} \langle u_Q^2 \rangle$$

Because $\langle |\mathbf{u}|^2 \rangle = \langle u_x^2 + u_y^2 + u_z^2 \rangle = 3 \langle u_x^2 \rangle = \langle u_Q^2 \rangle$

Schematic inelastic X-ray spectrum



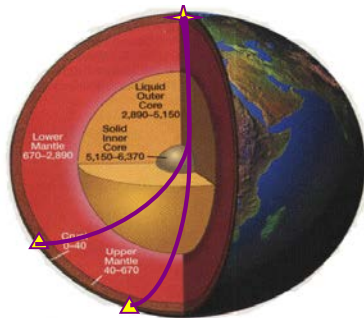
INELASTIC X-RAY SCATTERING

- High energy resolution studies of collective motion in solids and liquid phases
- Simultaneous information on energy E and momentum Q transferred between the photons and the electronic systems of interest

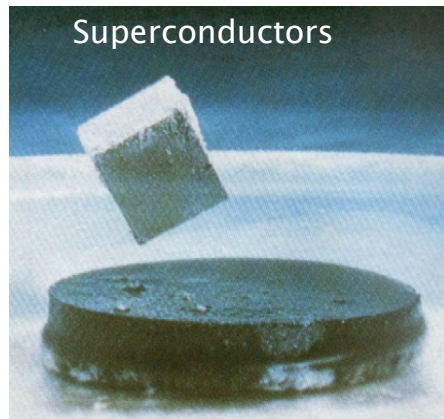
- Energy transfer: $E_i - E_f = \Delta E = 1 \text{ meV} - 200 \text{ meV}$
- Momentum transfer: $\Delta k = 1 - 180 \text{ nm}^{-1}$

- Phonon dispersion in single crystals with small sample volume
- Collective dynamics in disordered systems
- Phonon dispersion in geophysical relevant materials
- Lattice dynamics in thin films and interfaces

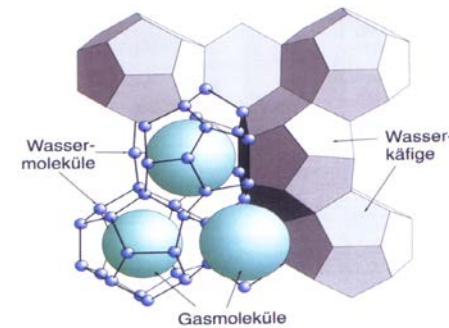
Sound velocities and elasticity



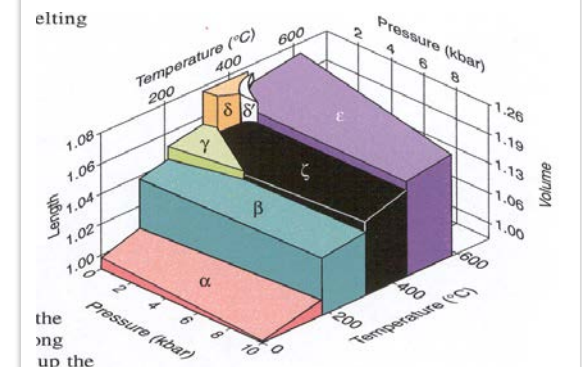
Superconductors



Thermal Conductivity



Phase stability



EX.: PHONON DISPERSION CURVES

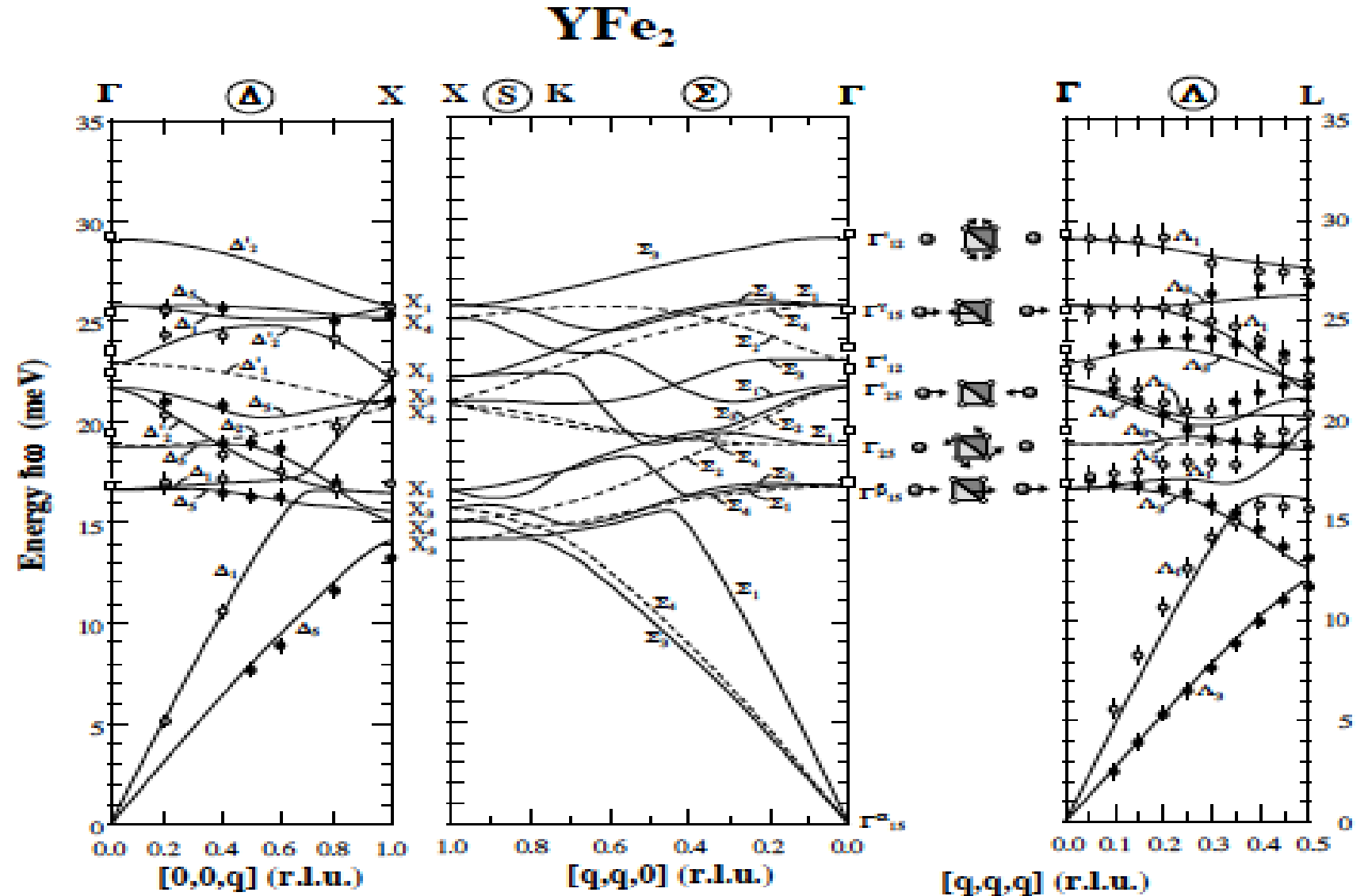
YFe₂ cubic Laves phase

2 formula unit
N= 6 atoms

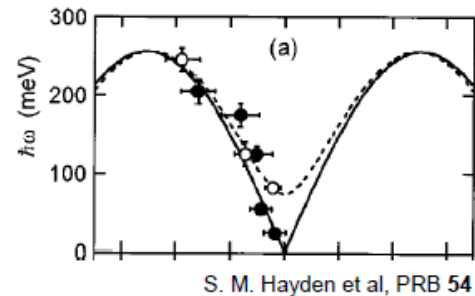
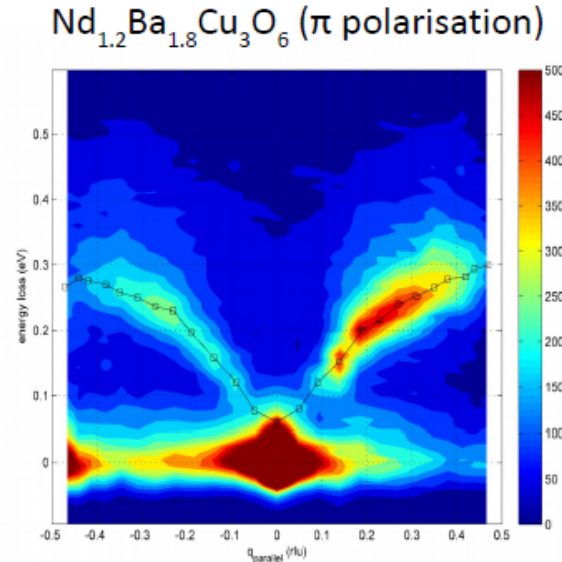
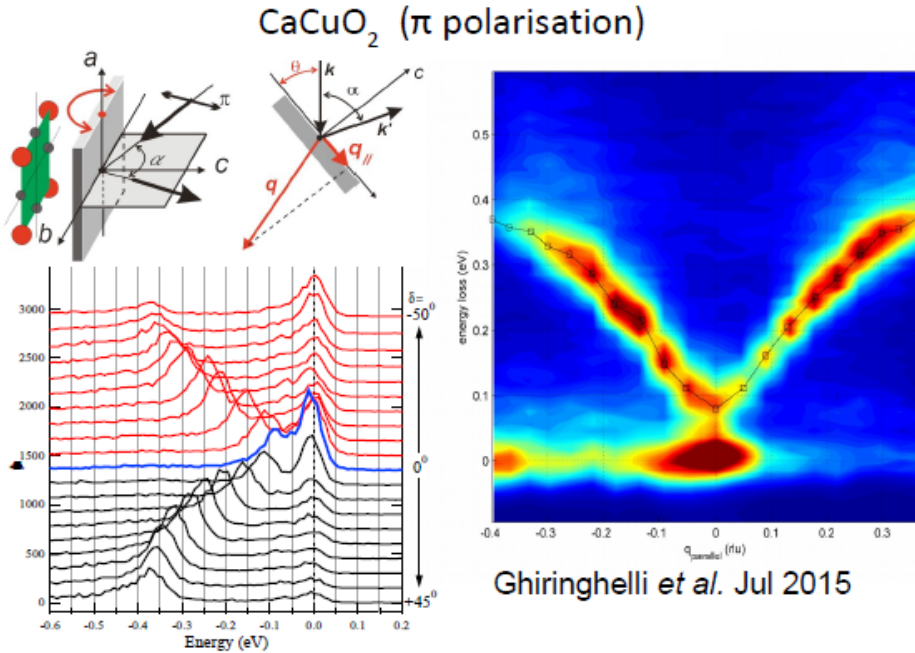
Phonon branches:
N x 3= 18 branches

3 acoustic:
1 long., 2 transv.

15 optics:
10 transverse
5 longitudinal



Magnon Dispersion



The sample used in INS was a single crystal of YBa₂Cu₃O_{6.15} with mass 96 g.

Inelastic Neutron Scattering:
 96 g (15.2 cm³) bulk crystal YBa₂Cu₃O_{6.15}

Resonant Inelastic X-ray Scattering:
 100 nm film crystal Nd_{1.2}Ba_{1.8}Cu₃O₆

Long-term collaboration between Politecnico di Milano and ESRF



POLITECNICO MILANO 1863



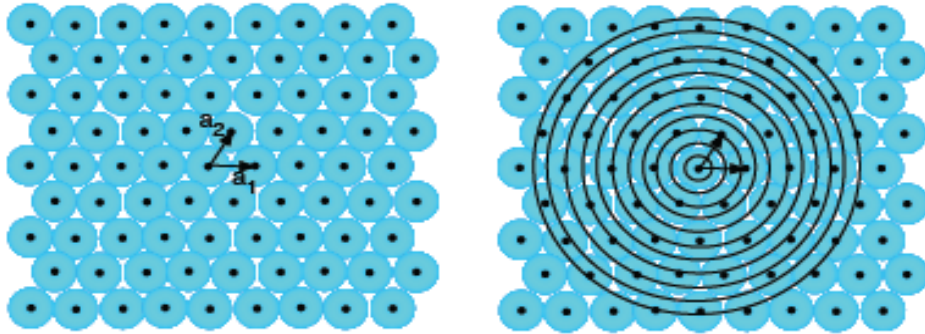
The European Synchrotron

Samples mass ratio: ~ 250 000

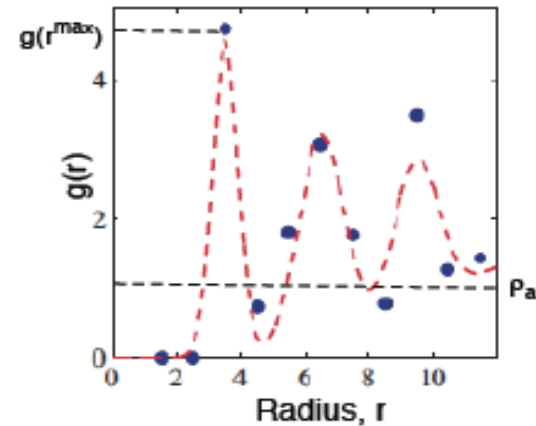
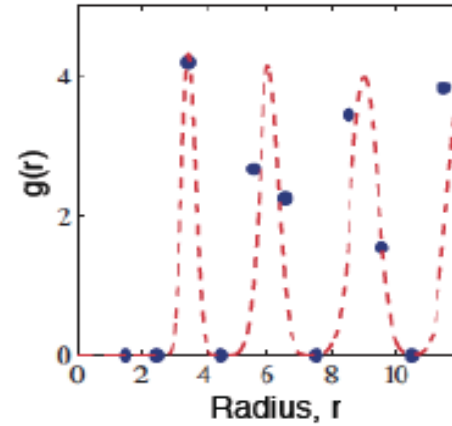
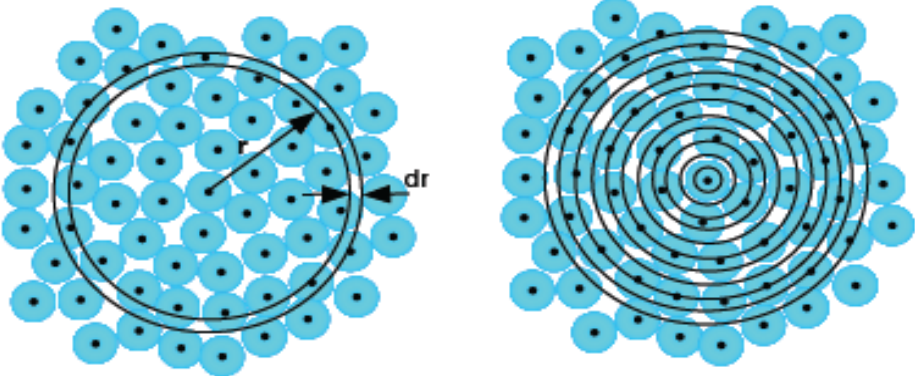
Scattering in non-crystalline materials

NON CRYSTALLINE MATERIALS

A) Crystalline material



B) Non-crystalline material



Radial distribution function:

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

Radial electronic density:

$$\rho(r)^{2D} = \frac{N(r)}{2\pi r dr}$$

$$\rho(r)^{3D} = \frac{N(r)}{4\pi r^2 dr}$$

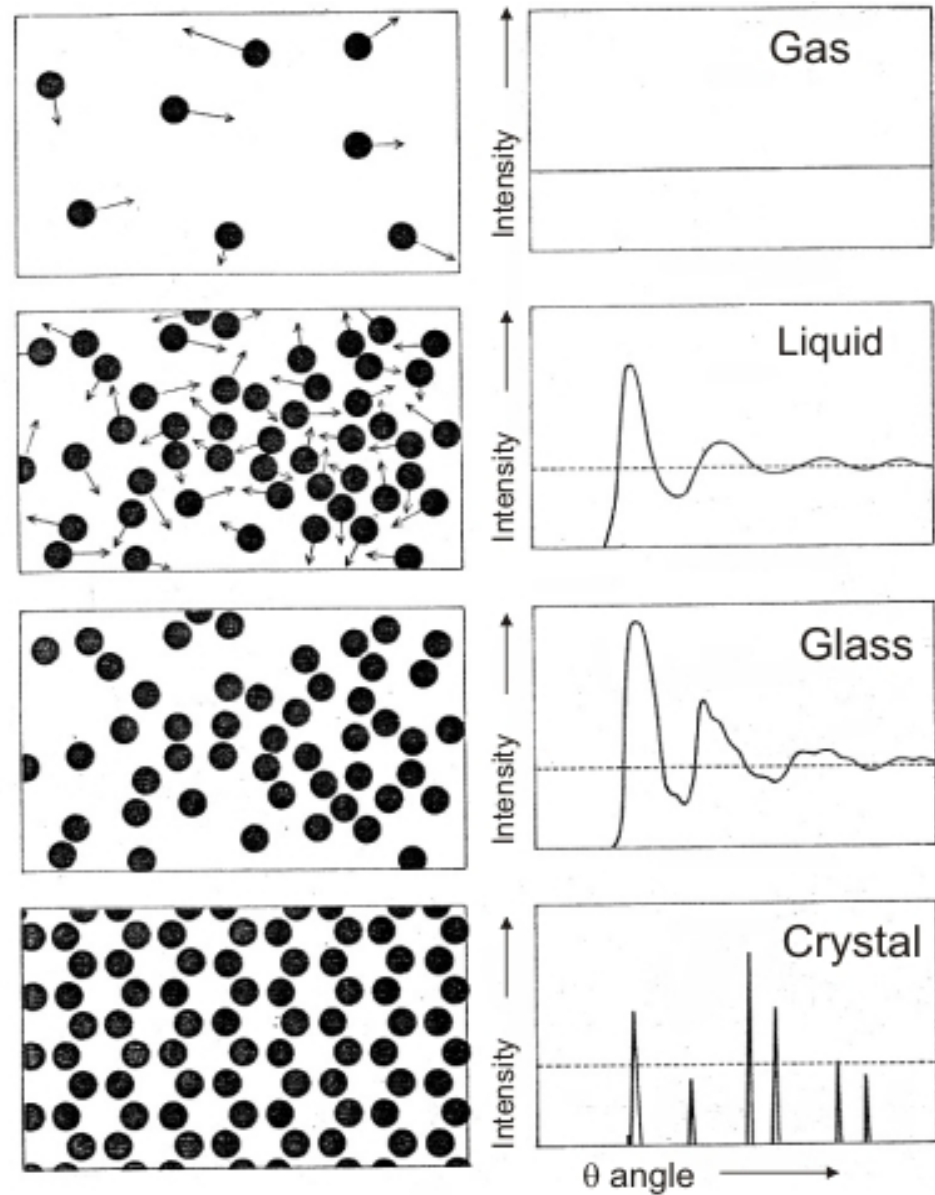
Averaged areal el. density

ρ_{at}

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

The radial distribution function $g(r)$ is the FT of the scattered intensity $I(Q)$.

SCATTERING INTENSITIES : FROM GAS TO SOLIDS



SCATTERING OF GLASSES AND LIQUIDS

$$\begin{aligned}
 I(Q) = & \overbrace{N f^2(Q) + f^2(Q) \sum_n \int_V [\rho(\mathbf{r}_{nm}) - \rho_{at}] e^{i\mathbf{Q} \cdot \mathbf{r}_{nm}} dV_m}^{\text{Short range order } I^{\text{SRO}}} \\
 & \underbrace{+ f^2(Q) \sum_n \int_V [\rho_{at}] e^{i\mathbf{Q} \cdot \mathbf{r}_{nm}} dV_m}_{\text{Small angle scattering } I^{\text{SAXS}}}
 \end{aligned}$$

Scattering intensity

Deviation of the electron density between two different scattering centers with respect to the averaged electron density

$$(\rho_n(\mathbf{r}_{nm}) - \rho_{at})$$

electron density at $\mathbf{r}_{nm}=(\mathbf{r}_n-\mathbf{r}_m)$ with respect at \mathbf{r}_n

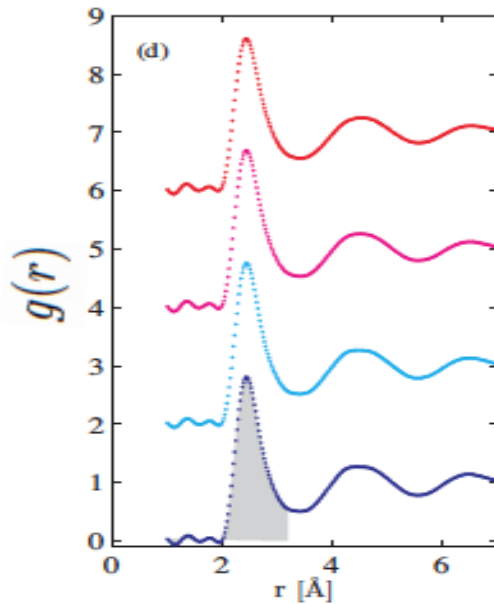
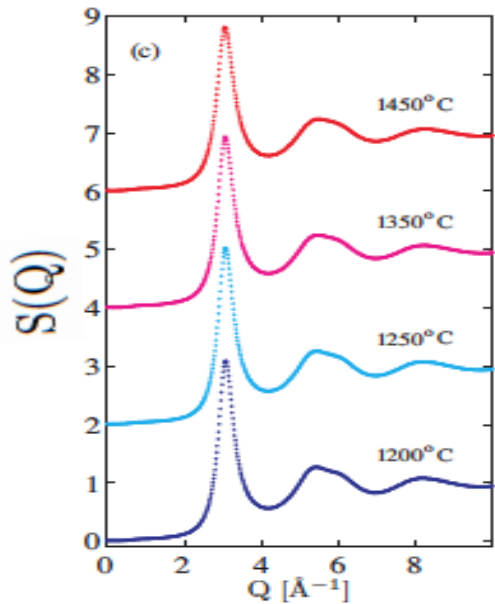
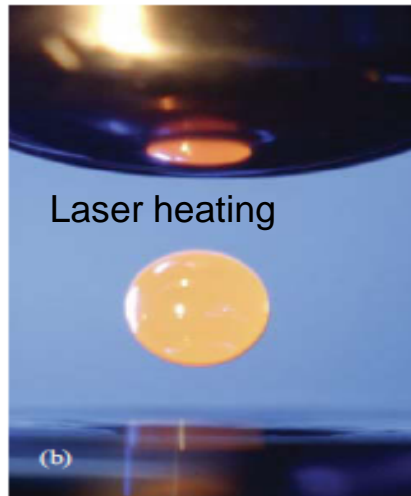
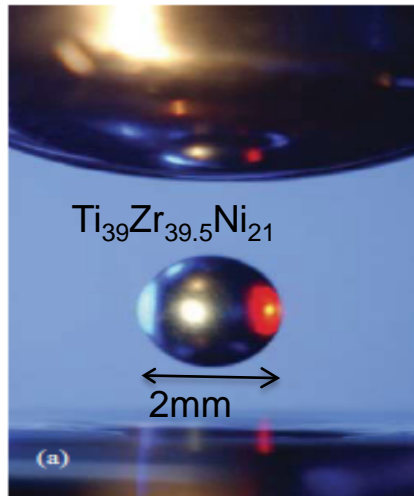
we add and subtract this term at the scattering intensity

I^{SRO} : Structural information on interatomic distances

I^{SAXS} : Information on shape. Morphology and size of molecular aggregate

EX.: LIQUID METALS

Electrostatic levitation



Liquid/glass “structure factor”

$$S(Q) = \frac{I^{SRO}(Q)}{Nf(Q)^2} = 1 + \frac{4\pi}{Q} \int_0^{\infty} r [\rho(r) - \rho_{av}] \sin(Qr) dr$$

Radial distribution function of Liquid/glass

$$g(r) = 1 + \frac{1}{2\pi^2 r \rho_{av}} \int_0^{\infty} Q [S(Q) - 1] \sin(Qr) dQ$$

The peak position indicate the first neighbour distance $r=2.5 \text{ \AA}$

The integral of the first peak gives the number of the atoms in the first coordination shell

$$N_{nn} = \int_{r_1}^{r_2} \rho_{at} g(r) 4\pi r^2 dr$$

$N \sim 12$ nearest neighbours
Icosahedral coordination

SMALL ANGLE X-RAYS SCATTERING (SAXS)

Scattering at small Q vectors is sensitive to the uniform electron distribution in molecules of shaped large object (polymers, biological macro-molecules ...)

$$I^{saxs}(Q) = f^2(Q) \sum_n \int_V \rho_{at} e^{i\mathbf{Q} \cdot (\mathbf{r}_n - \mathbf{r}_m)} dV_m = \left| \int_V \rho_{sl} e^{i\mathbf{Q} \cdot \mathbf{r}_n} \right|^2$$

Scattering length density: $\rho_{sl} = f(Q) \rho_{at}$ Fourier transform of charge density

For diluted molecules in solutions:

$$I^{saxs}(Q) = (\rho_{slp} - \rho_{sl0}) \int_{V_p} e^{i\mathbf{Q} \cdot \mathbf{r}_n} dV_p$$

Particle scattering length density

Solvent scattering length density

Particle "form factor"

$$F(Q) = \frac{1}{V_p} \int_{V_p} e^{i\mathbf{Q} \cdot \mathbf{r}_n} dV_p$$

V_p particle volume

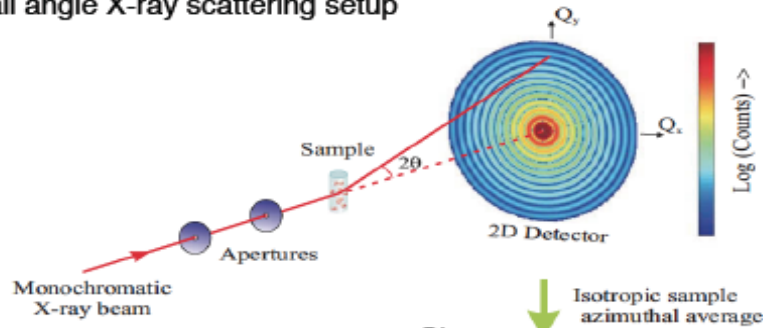
EX.: SAXS ON RIGID SPHERES

Small angle scattering experiment on a rigid sphere of radius R

$$I^{saxs}(Q) = \Delta\rho^2 V_p^2 |F(Q)|^2$$

$\Delta\rho$ = excess of number of electrons with respect to the solvent
 $F(Q)$ form factor of the sphere
 V_p =volume of the sphere

A) Small angle X-ray scattering setup



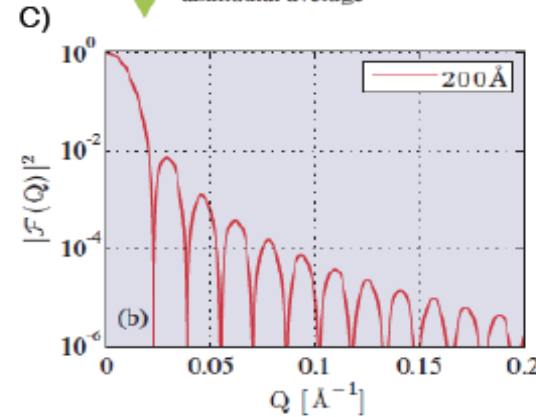
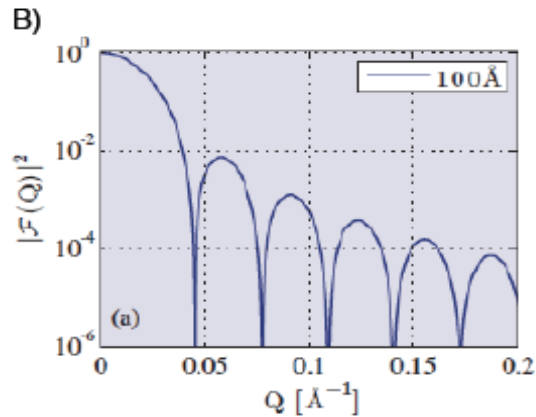
Form of the a sphere of radius R

$$\begin{aligned} F^{sphere}(Q) &= \frac{1}{V_p} \int_0^R \int_0^{2\pi} \int_0^\pi e^{iQr \cos\theta} r^2 \sin\theta d\theta d\phi dr \\ &= \frac{4\pi}{V_p} \int_0^R \frac{\sin(Qr)}{Qr} r^2 dr \\ &= 3 \left[\frac{\sin(QR) - QR \cos(QR)}{Q^3 R^3} \right] \\ &= \frac{3J_1(QR)}{QR} \end{aligned}$$

Long wavelength limit

$$QR \ll 1$$

$$I^{saxs}(Q) = \Delta\rho^2 V_p^2$$



PARTICLE DIMENSIONALITY

	$ \mathcal{F}(Q) ^2$	Radius of gyration R_g
Sphere ($d = 3$)	$\left(\frac{3J_1(QR)}{QR}\right)^2$	$\sqrt{\frac{3}{5}} R$
Disc ($d = 2$)	$\frac{2}{Q^2 R^2} \left(1 - \frac{J_1(2QR)}{QR}\right)$	$\sqrt{\frac{1}{2}} R$
Rod ($d = 1$)	$\frac{2Si(QL)}{QL} - \frac{4\sin^2(QL/2)}{Q^2 L^2}$	$\sqrt{\frac{1}{12}} L$

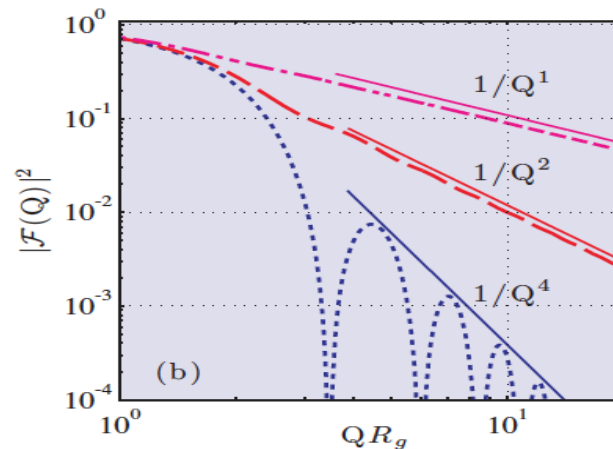
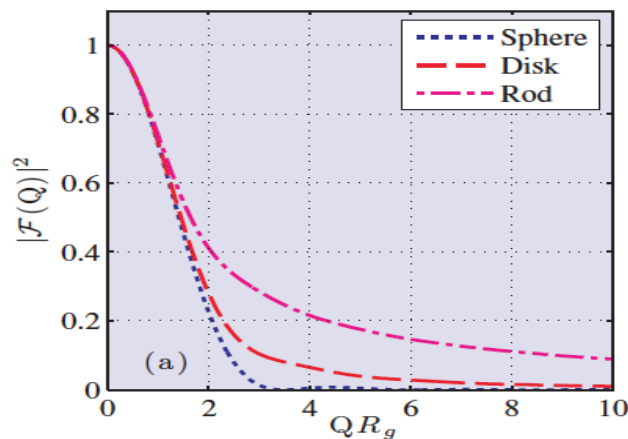
Radius of giration

$$R_g^2 = \frac{1}{V_p} \int_{V_p} r^2 dV_p$$

$$R_g^2 = \frac{\int_{V_p} \rho_{sl,p}(\mathbf{r}) r^2 dV_p}{\int_{V_p} \rho_{sl,p}(\mathbf{r}) dV_p}$$

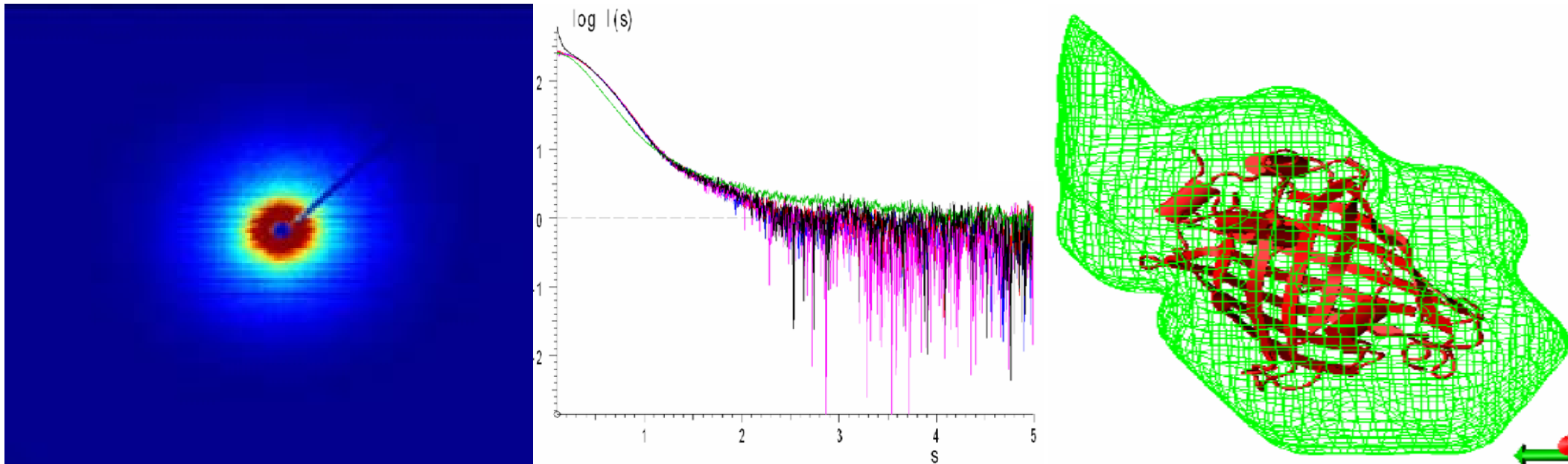
Uniform sphere

$$I_1^{SAXS}(Q) \approx \Delta\rho^2 V_p^2 e^{-Q^2 R_g^2/3}$$



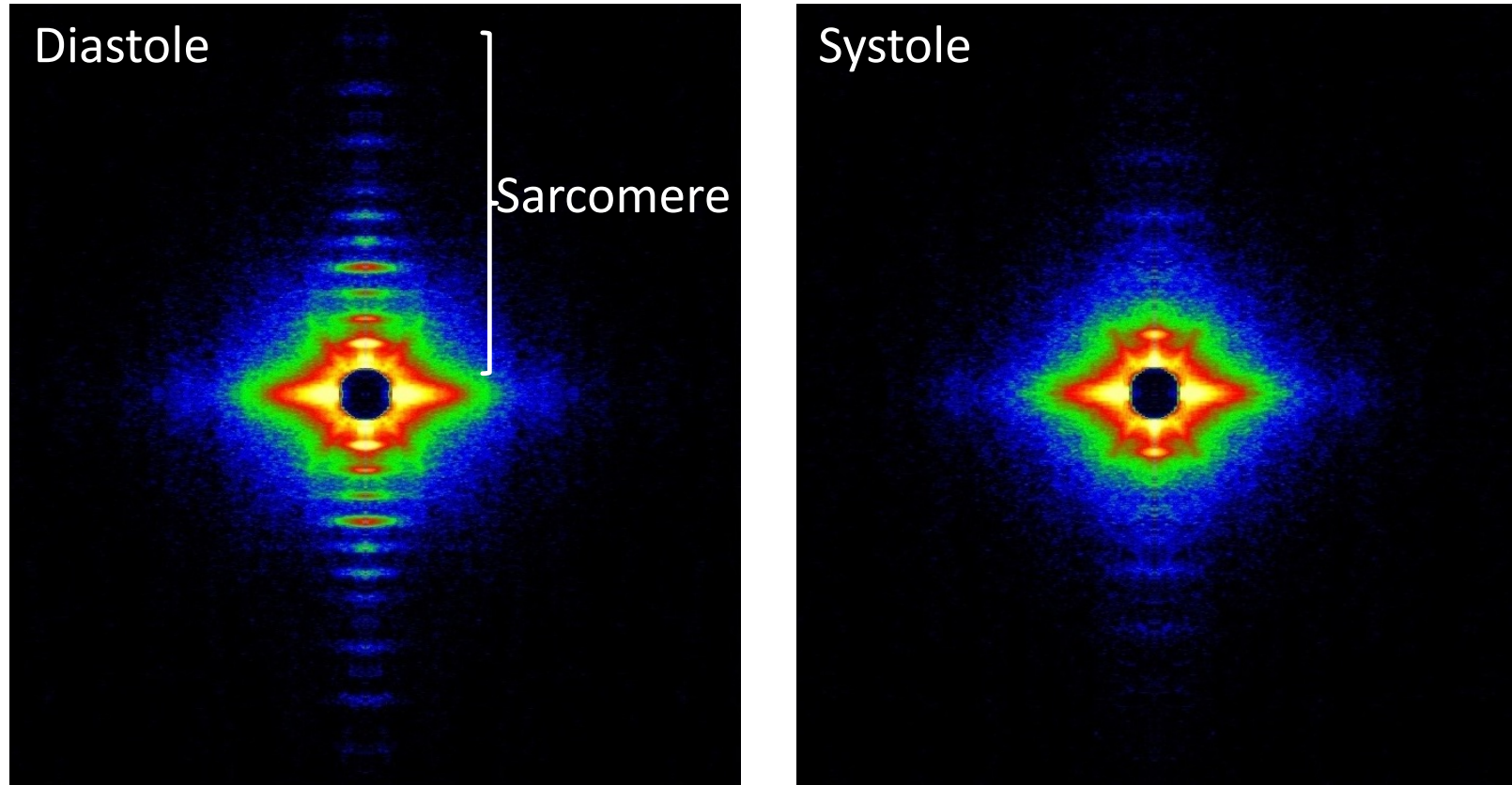
Small Angle X-ray Scattering (SAXS) is a technique for studying structure at low resolution in solution & under normal biophysical/biochemical conditions

- Information from SAXS:**
- model independent parameters (R_g , $I(0)$)
 - *ab initio* shape determination
 - rigid body modelling



molecular shape, molecular interactions, kinetics, etc...

Ultra low angle diffraction reveals changes at the sarcomere (unit cell) during the activation and probe the supramolecular organization within

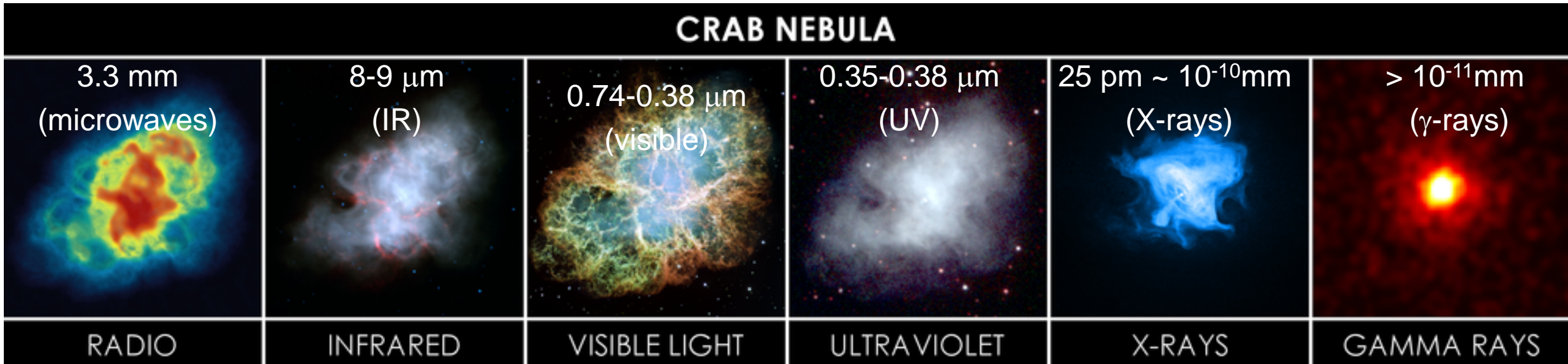


Allows to derive the force-sarcomere length relationship and to observe significant changes in the supramolecular organization

X-rays absorption

PHOTON ABSORPTION/EMISSION

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

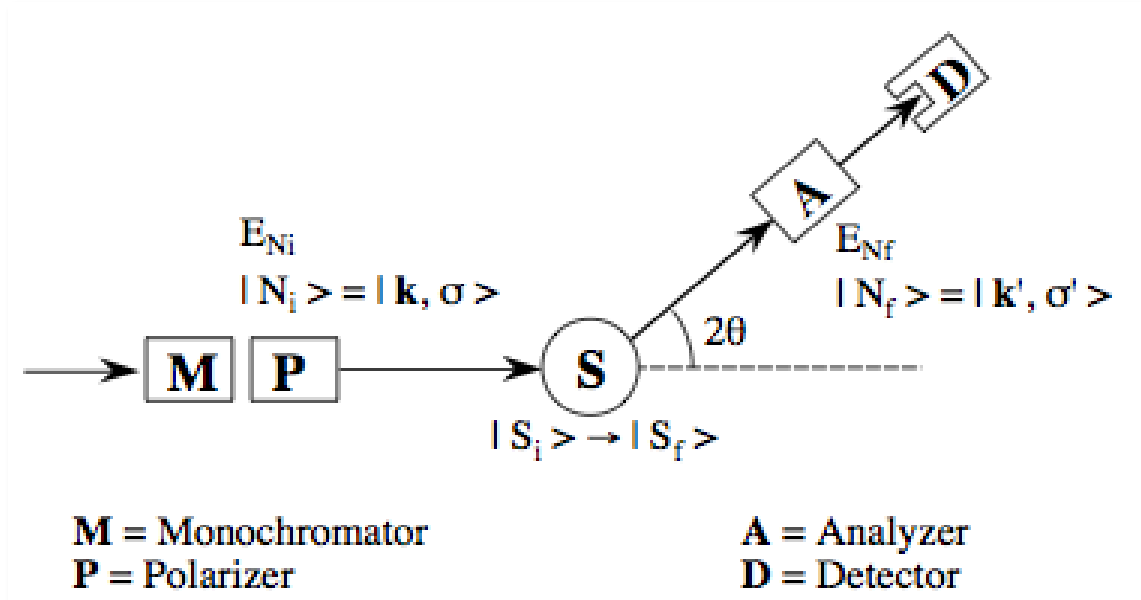


The crab nebula in radio, infrared, visible, ultraviolet, x-ray and gamma-ray wavelengths.

Sources: Radio: NRAO/AUI and M. Bietenholz, J.M. Uson, T.J. Cornwell; Infrared: NASA/JPL-Caltech/R. Gehrz (University of Minnesota); Visible: NASA, ESA, J. Hester and A.Loll (Arizona State University); Ultraviolet: NASA/Swift/E. Hoversten, PSU, X-ray: NASA/CXC/SAO/F. Seward et al.; Gamma: NASA/DOE/Fermi LAT/R. Buehler

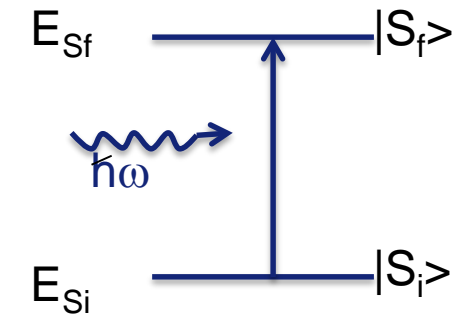
FERMI'S GOLDEN RULE

The aim of a scattering experiment is the determination of temporal evolution of the physical state of a large number of particle at the thermal equilibrium.



Dynamical variables

E_N probe energy
 σ spin or polarization
 k wavevector



Fermi's Golden rule

Transition probability (per unit time) from an initial $|S_i N_i\rangle$ and a final state $|S_f N_f\rangle$ of the system $|sample+probe\rangle$, related to the interaction potential V :

$$W_{N_i S_i N_f S_f} = \frac{2\pi}{\hbar} \sum_{S_i S_f} |\langle S_f N_f | V | S_i N_i \rangle|^2 \delta(E_{S_i} + E_{N_i} - E_{S_f} - E_{N_f})$$

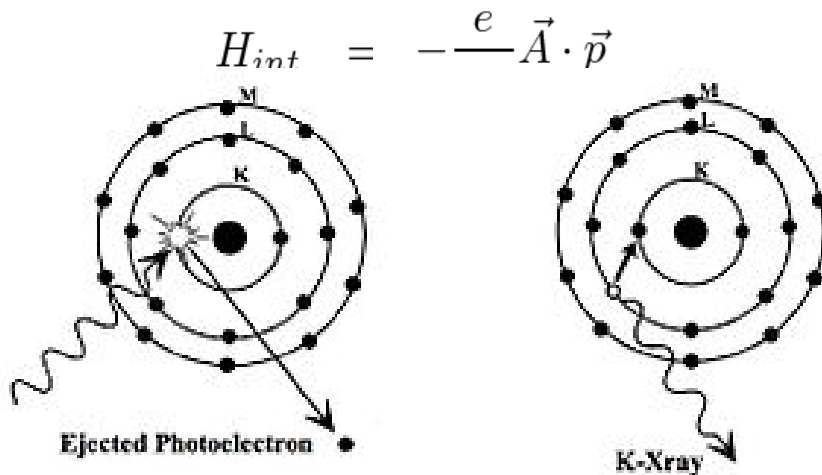
The interaction Hamiltonian is the weak relativistic limit of Dirac's equation (terms $v/c < 1$)

$$H = \frac{1}{2m} \left(\vec{p} + \frac{e}{c} \vec{A} \right)^2 + V(r)$$

$$H_{int} = -\frac{e}{2mc} (\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}) + \frac{e^2}{2mc^2} \vec{A} \cdot \vec{A}$$

$$= -\frac{e}{mc} \vec{A} \cdot \vec{p} + \frac{e^2}{2mc^2} \vec{A} \cdot \vec{A}$$

Absorption and emission processes



Scattering processes

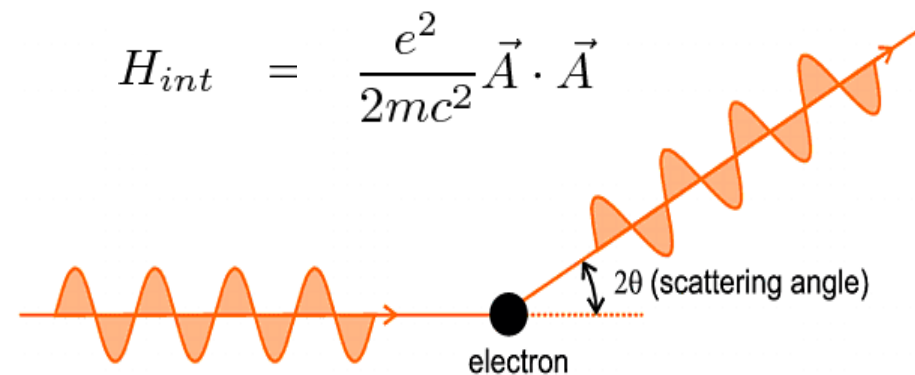
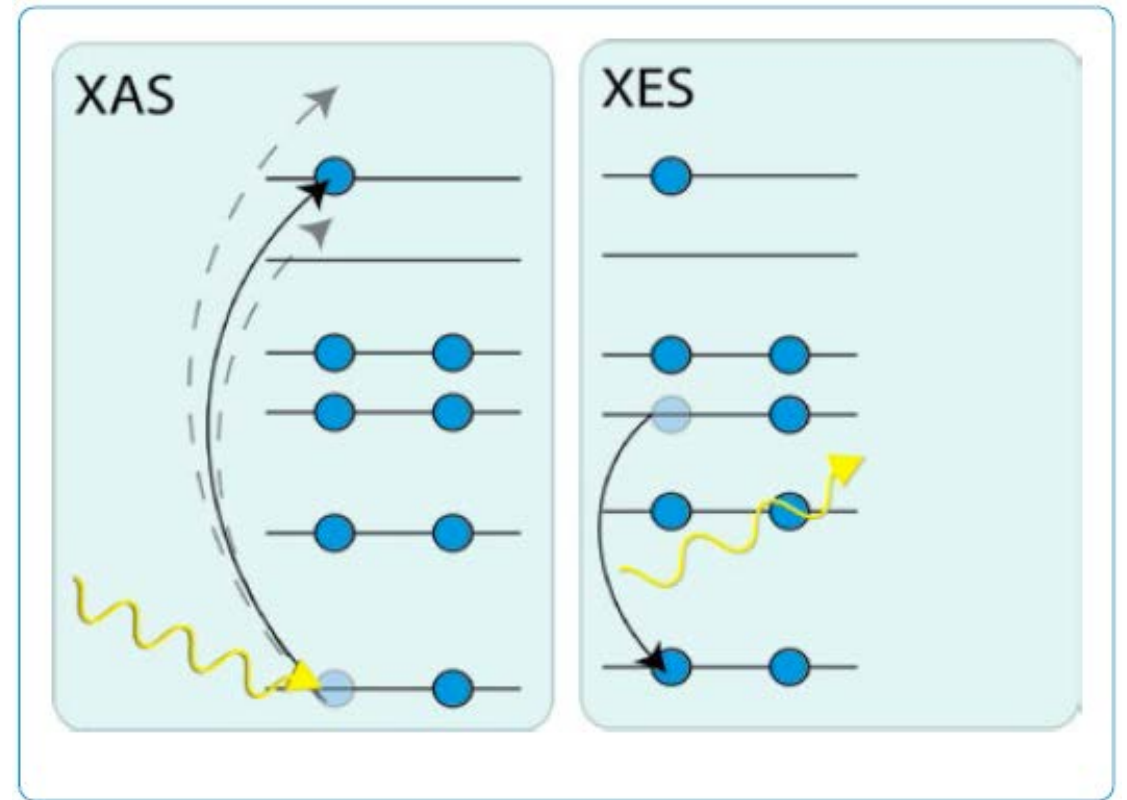
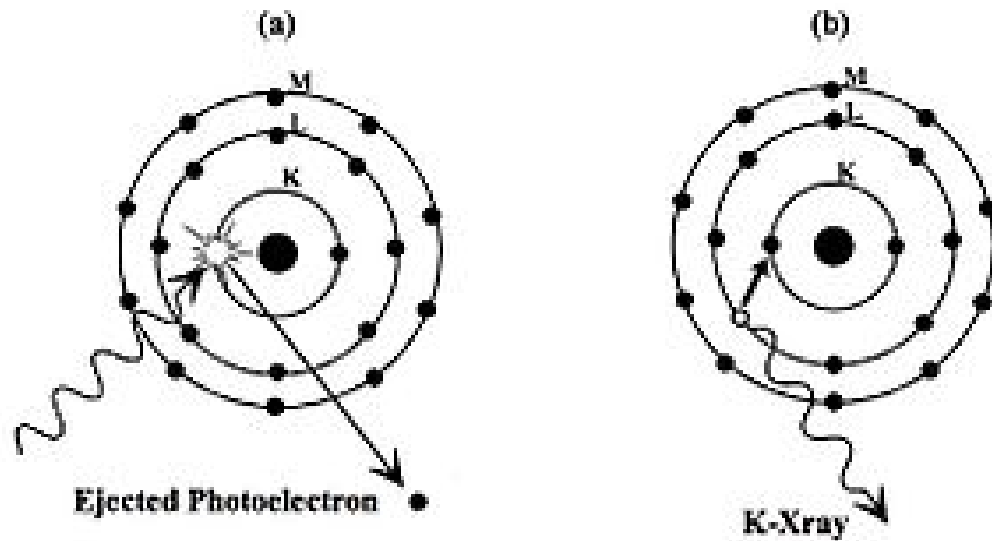


PHOTO-ELECTRON ABSORPTION AND EMISSION PROCESSES

Absorption and emission processes of photo-electrons probe the atomic level and valence orbital symmetries of the material under investigation.

$$H_{int} = -\frac{e}{mc}\vec{A} \cdot \vec{p}$$

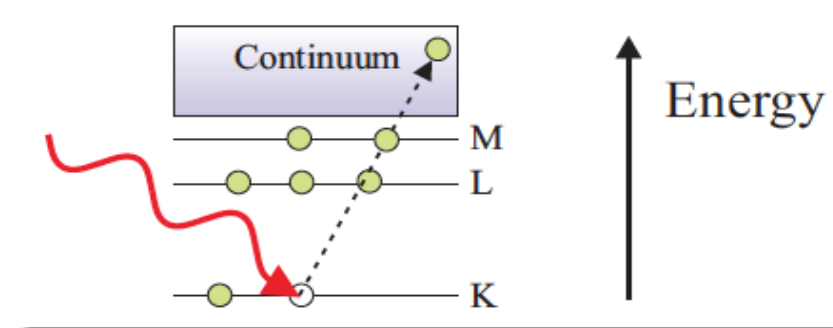


ABSORPTION AND EMISSION PROCESSES

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

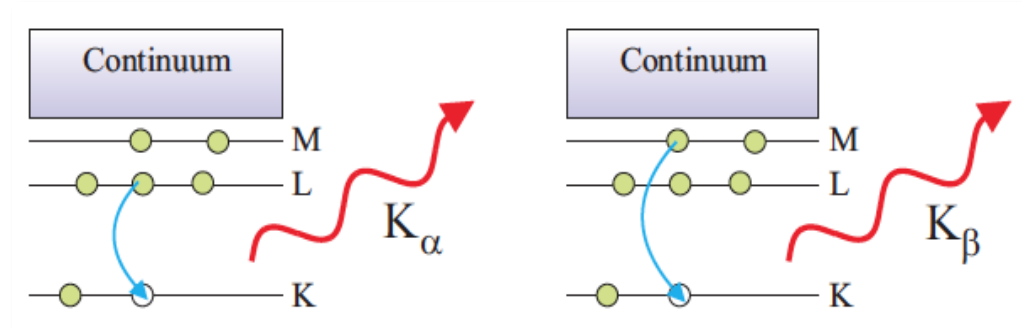
Photo-electric absorption

Photon absorbed and electron emitted in the continuum



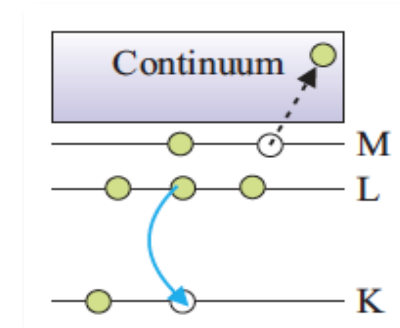
Fluorescent emission

An electron from the outer shell fill the hole and emit a photon



Auger electron emission

The atom relax into the ground state by emitting an electron

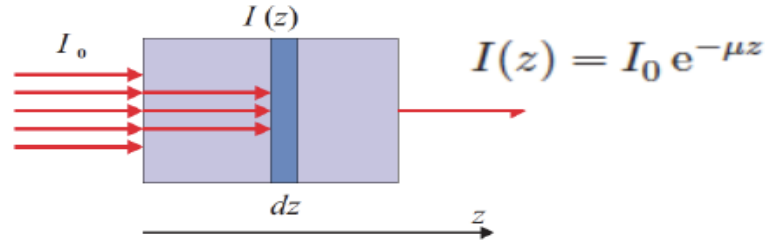


X-RAY ABSORPTION EDGES

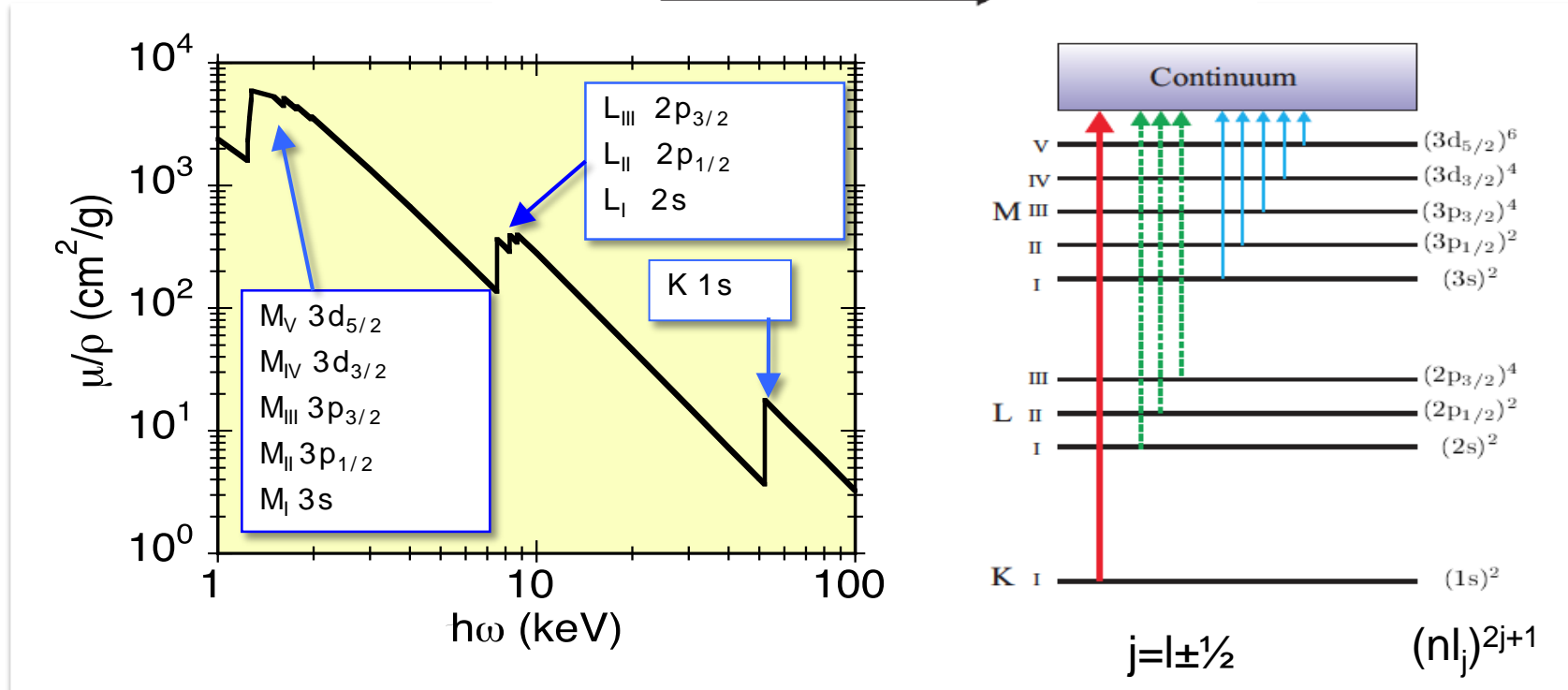
X-rays energies are able to extract atomic electrons from the atomic core.

The **element-specific** energies of the discontinuous jumps in the x-rays absorption spectra are called absorption edges.

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

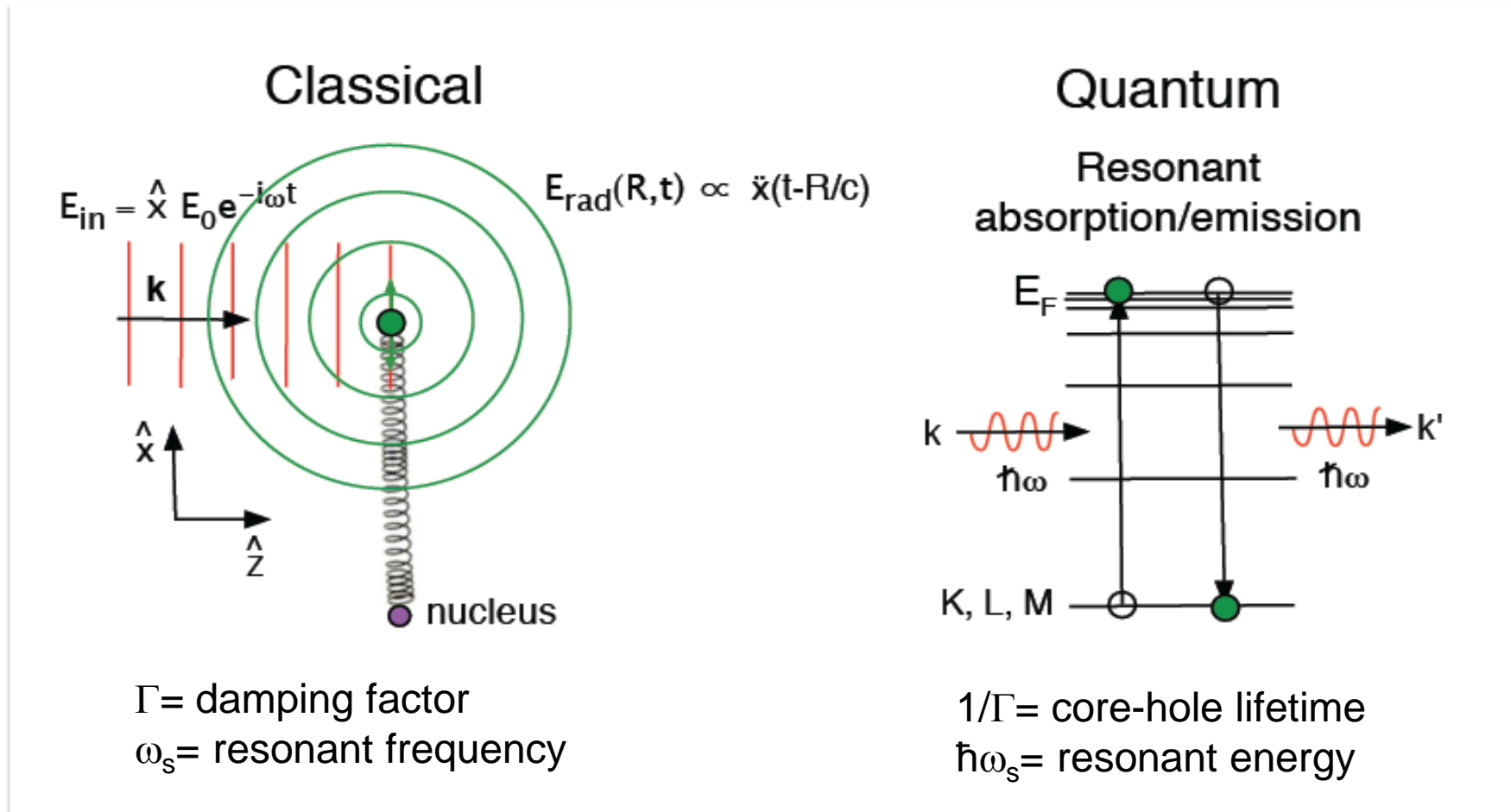


$$\sigma_{abs} \propto (h\omega)^{-3} Z^4$$



SCATTERING FROM BOUND ELECTRONS

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



THE CLASSICAL FORCED OSCILLATOR

The amplitude of the forced oscillations:

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

Γ = damping factor

ω_s = resonant frequency

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

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

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

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

Thomson term
(Q dependence)

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

Absorption correction
(dissipation term)

X-RAY ABSORPTION AND DISPERSION CORRECTIONS

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”.

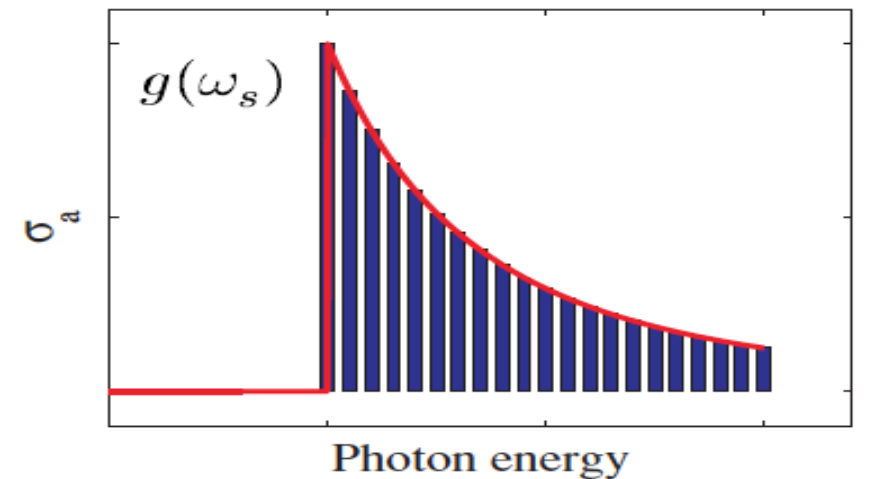
$$f(\mathbf{Q}, \omega) = f^0(\mathbf{Q}) + f'(\omega) + i f''(\omega)$$

Thomson term
(Q dependence)

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

Absorption correction
(dissipation term)

The absorption cross section σ_a is a superposition of oscillators with relative weights, so-called oscillator strengths, $g(\omega_s)$, proportional to $\sigma_a(\omega = \omega_s)$.



SCATTERING AND REFRACTIVE INDEX

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 .

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

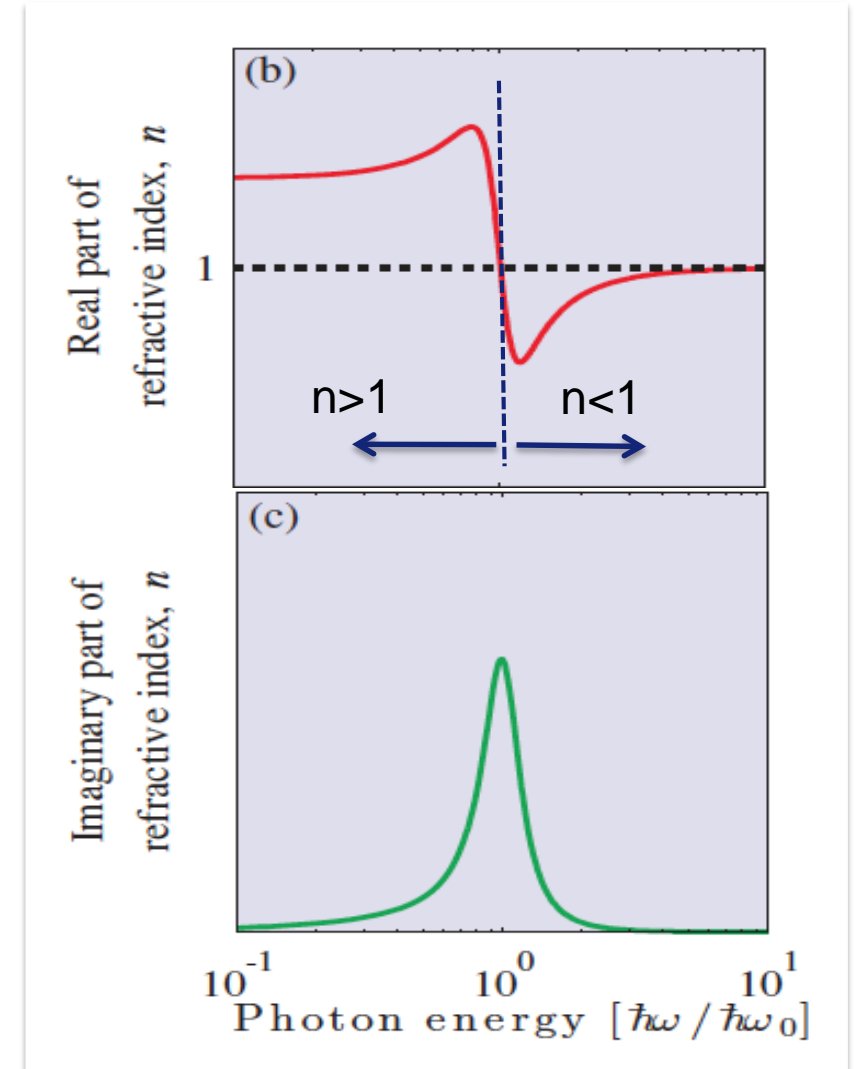
For $\omega \ll \omega_s \Rightarrow n > 1$ visible light

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

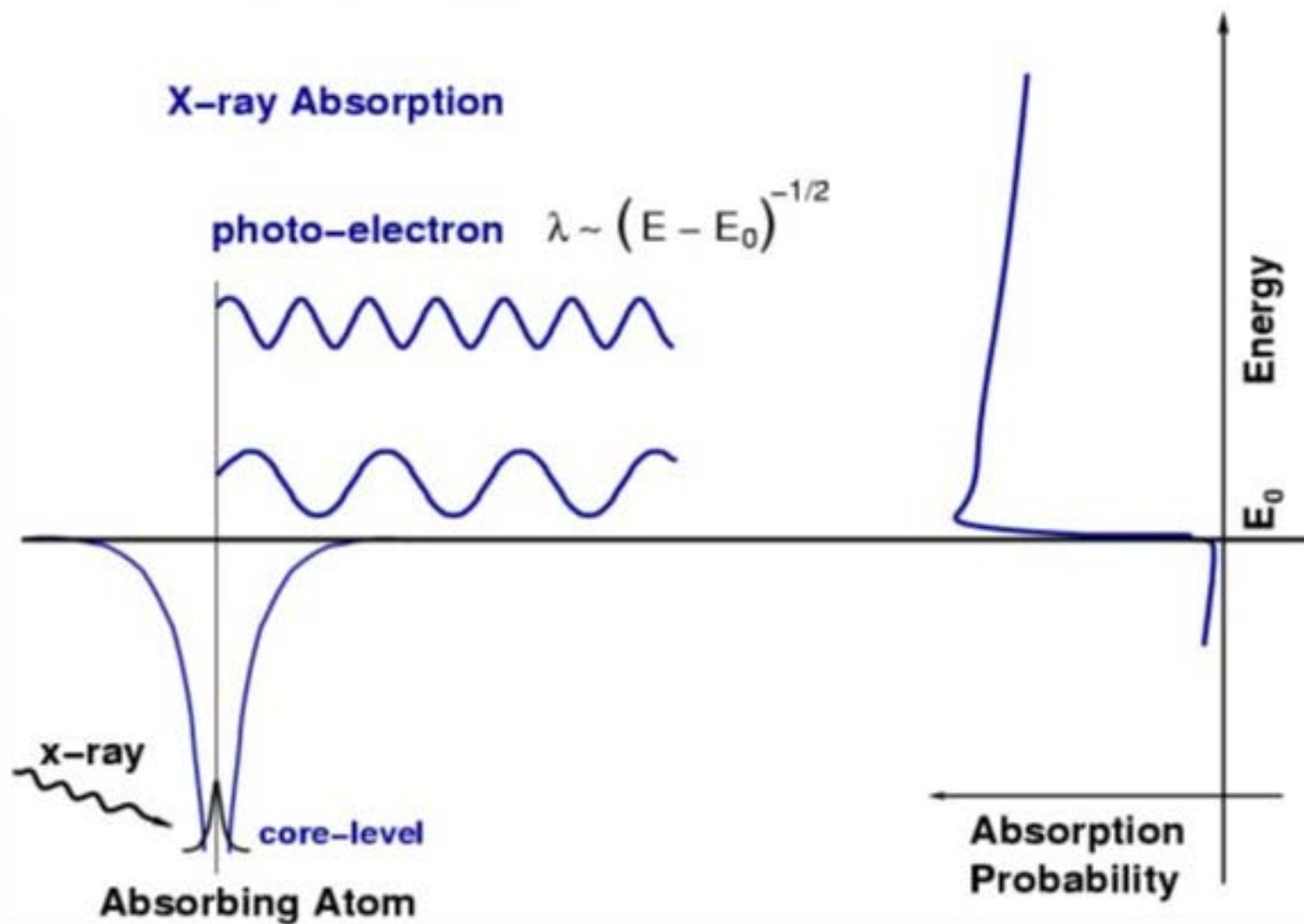
Notice that if $\omega \gg \omega_s \gg \Gamma$

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

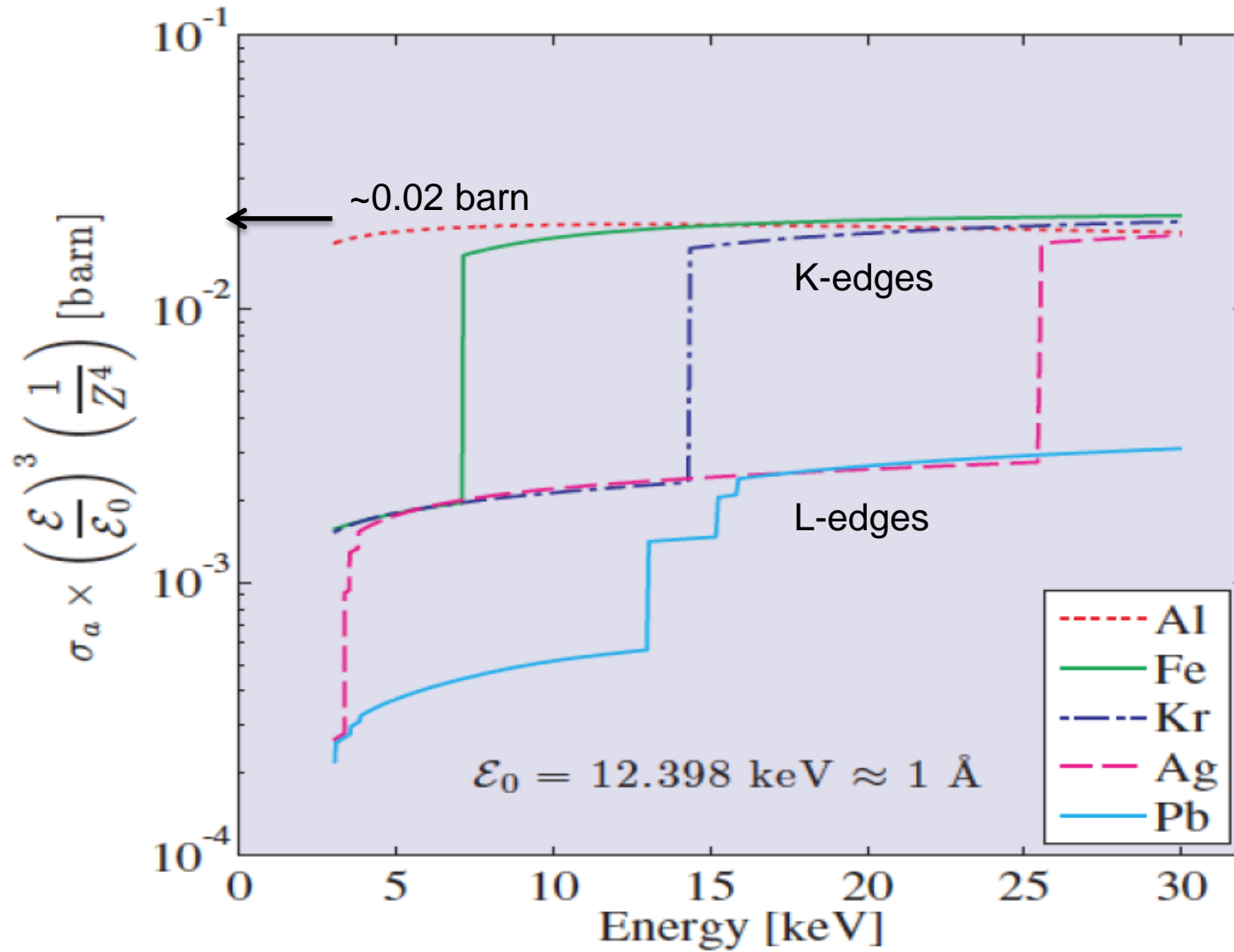
Real part of refractive index



ABSORPTION OF AN ISOLATED ATOM

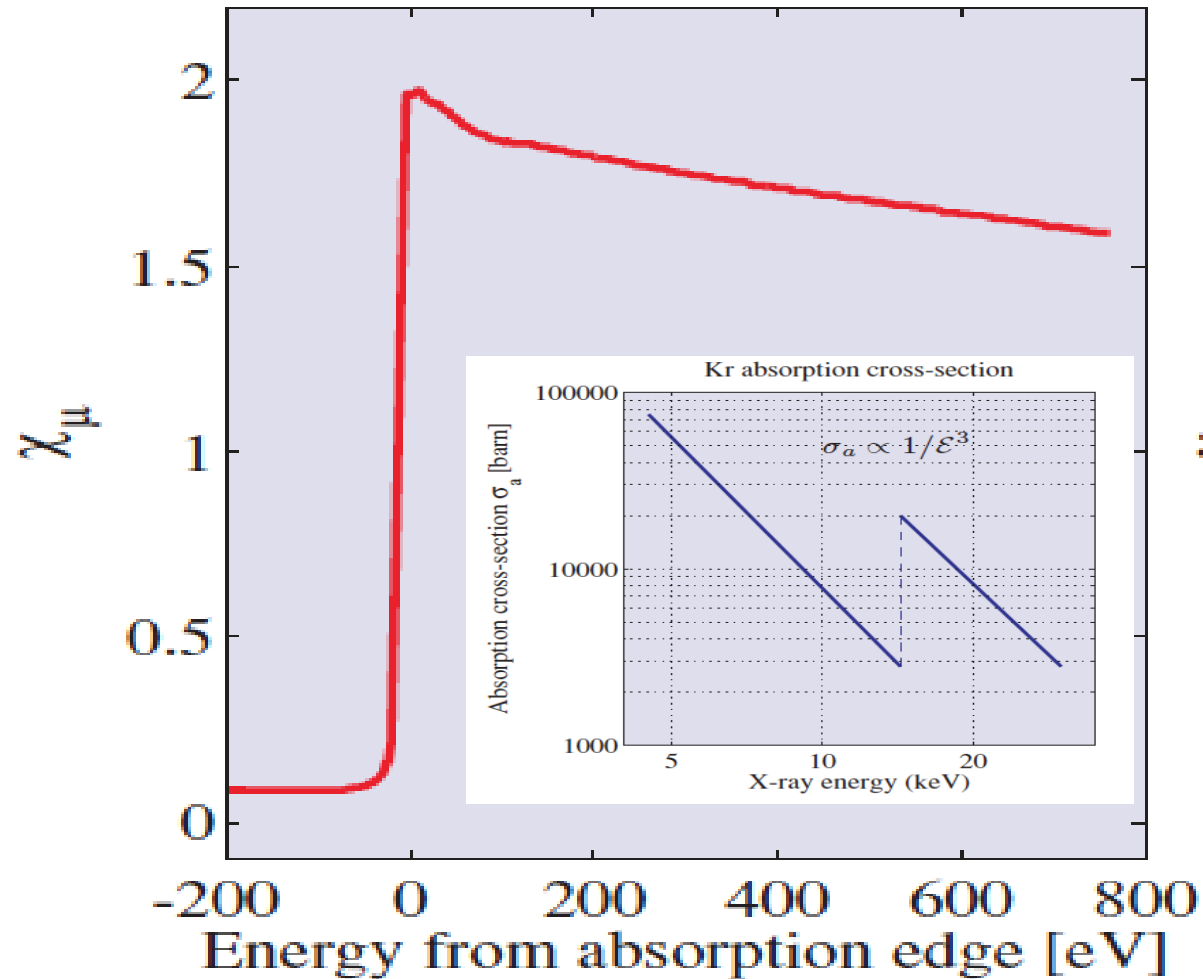


EXPERIMENTAL RESULTS K-EDGES

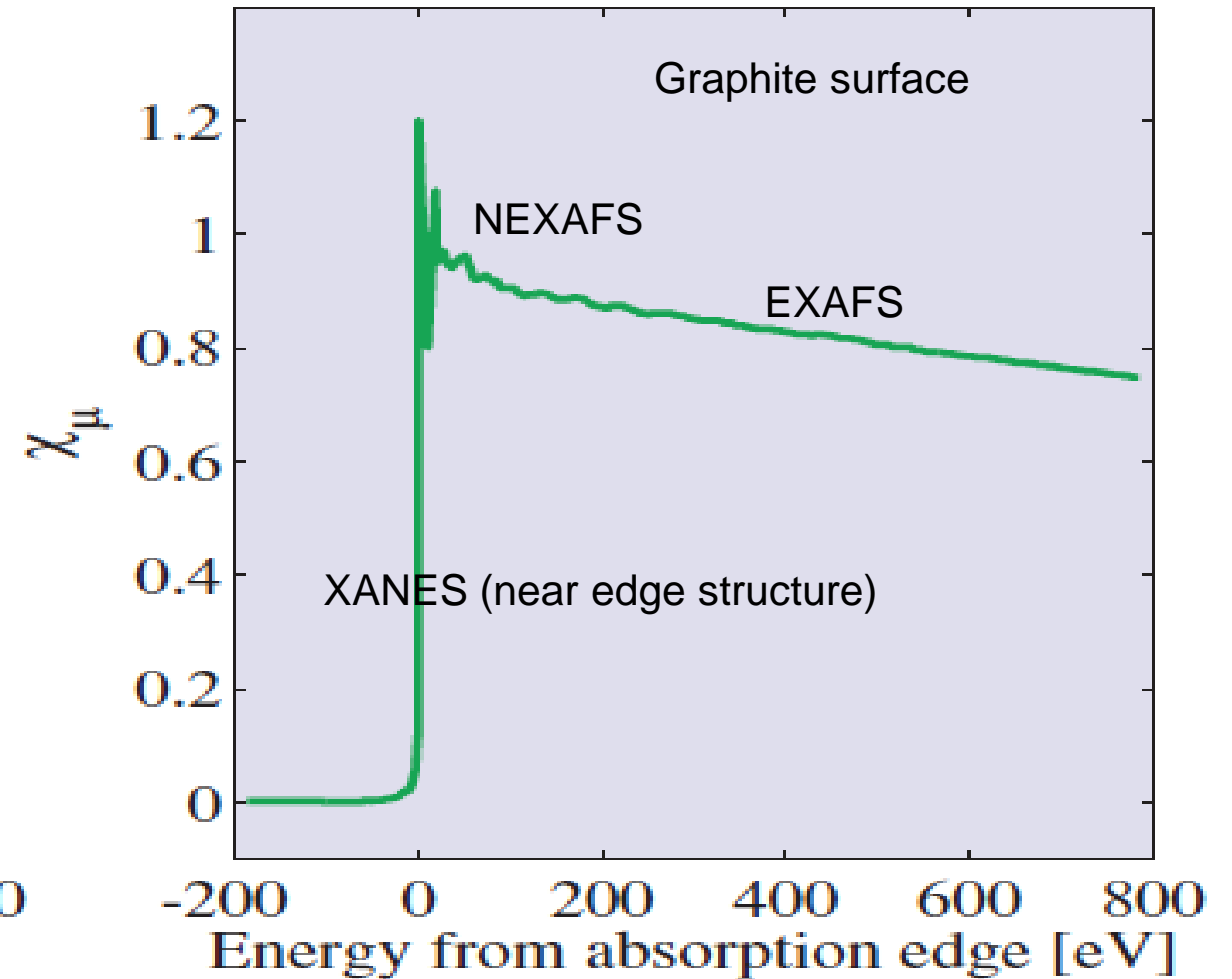


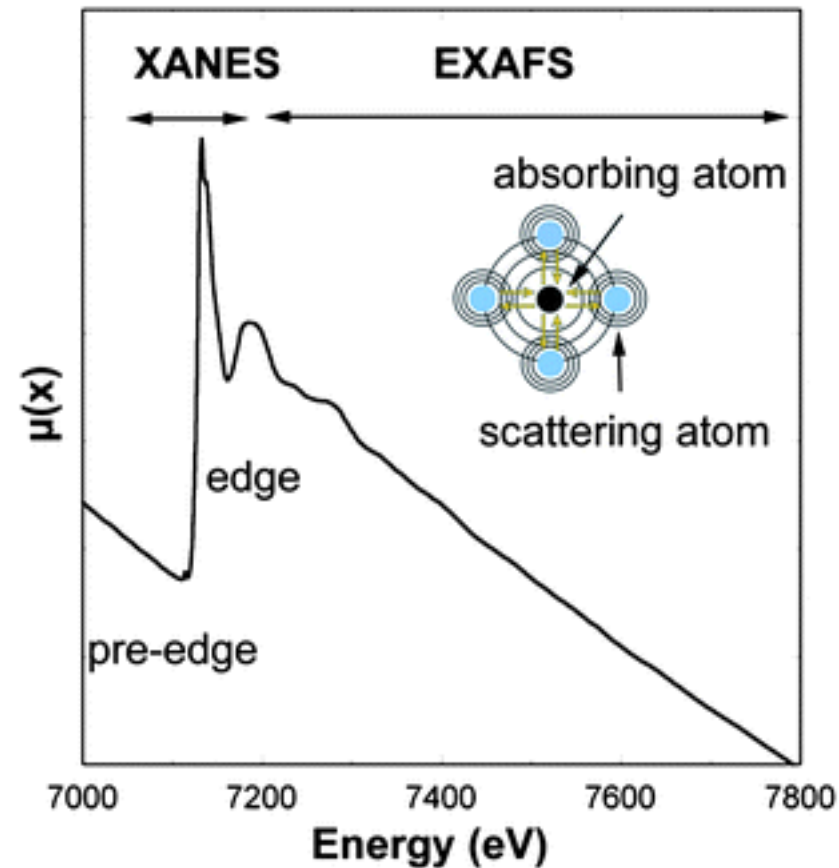
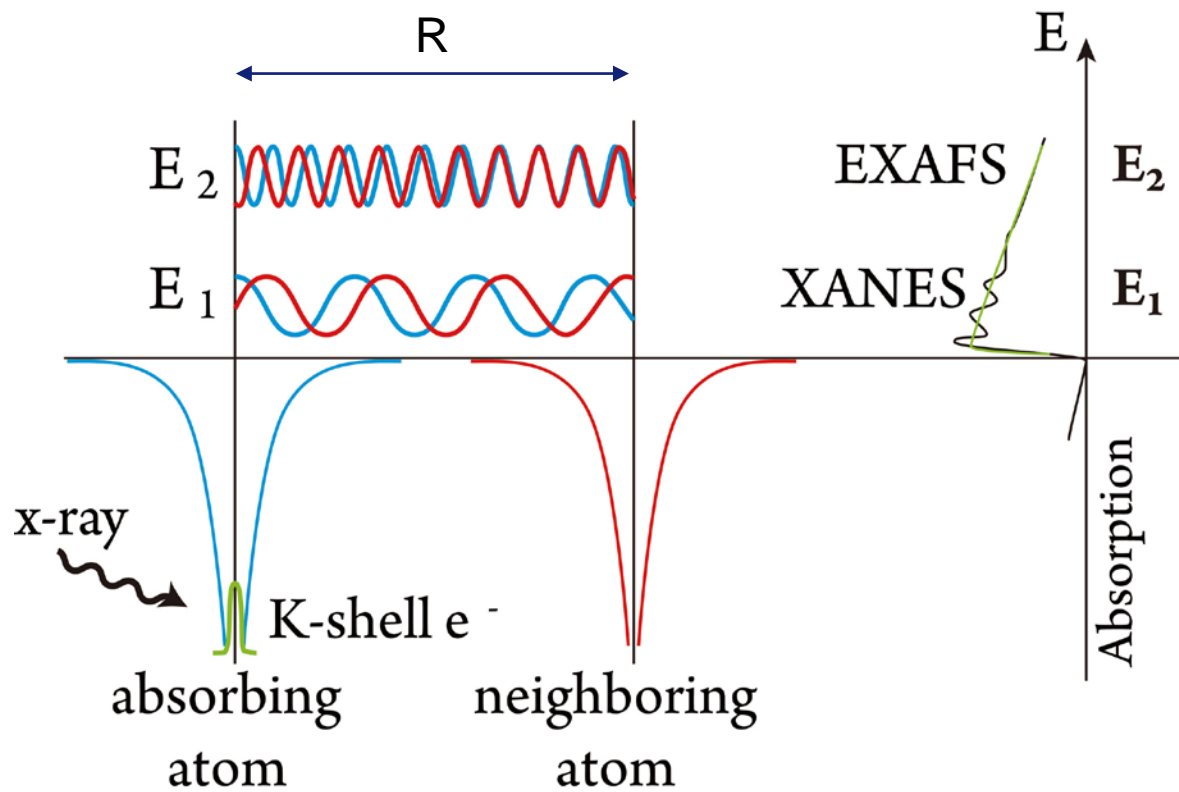
ABSORPTION IN GAS AND CRYSTALLINE MATERIALS

Kr gas



2D crystalline Kr

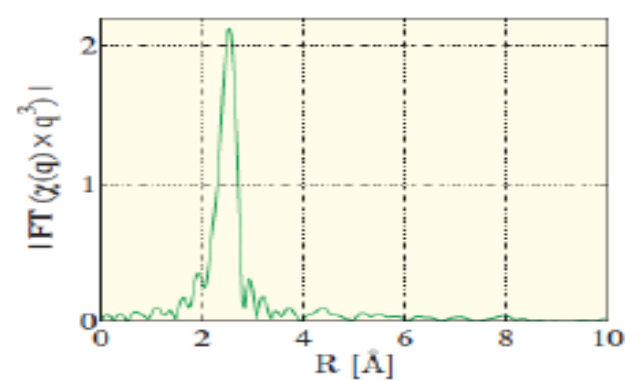
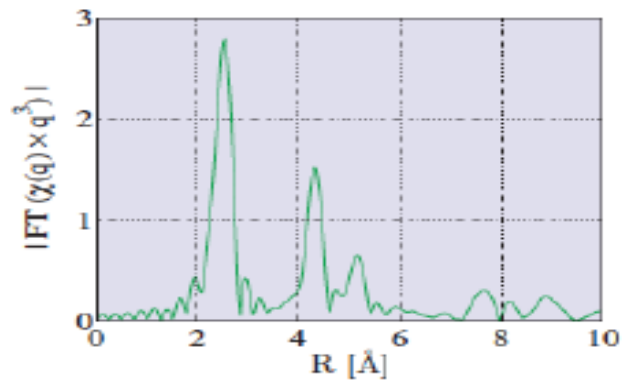
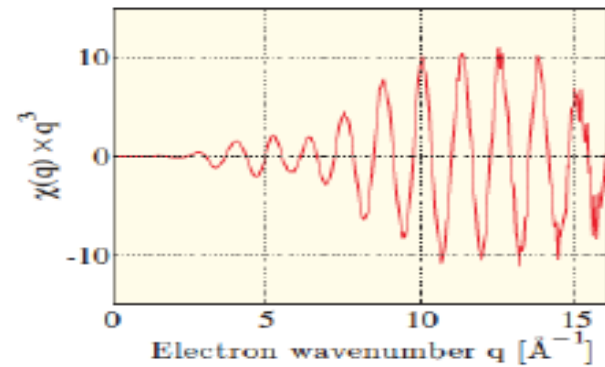
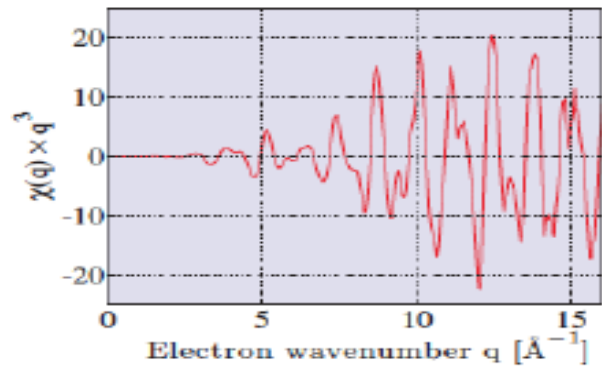
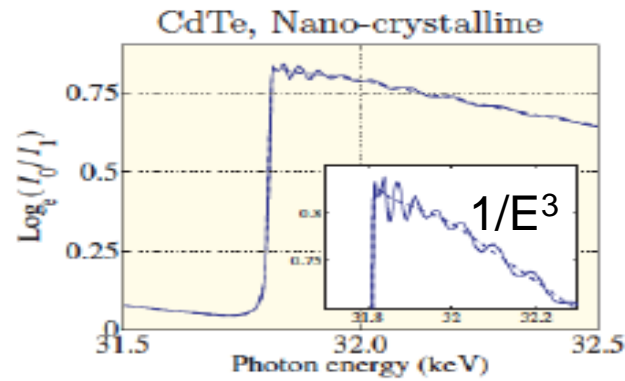
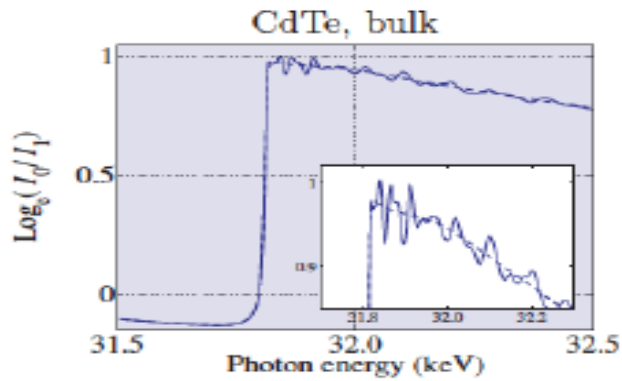




$$\psi_{backscatt.}(0) = t(q) \frac{e^{i(2qR+\delta)} + c.c.}{qR^2}$$

$2R$ = double distance (neighbour)-(absorbing atom)
 $t(q)$ = scattering amplitude of neighbour atom
 δ = phase shift

EXAMPLE: CdTe NANO-CRYSTALS - I



Te K-edge

Nano-crystals:

$N=3.55$

Only first neighbours
(reduced clusters)

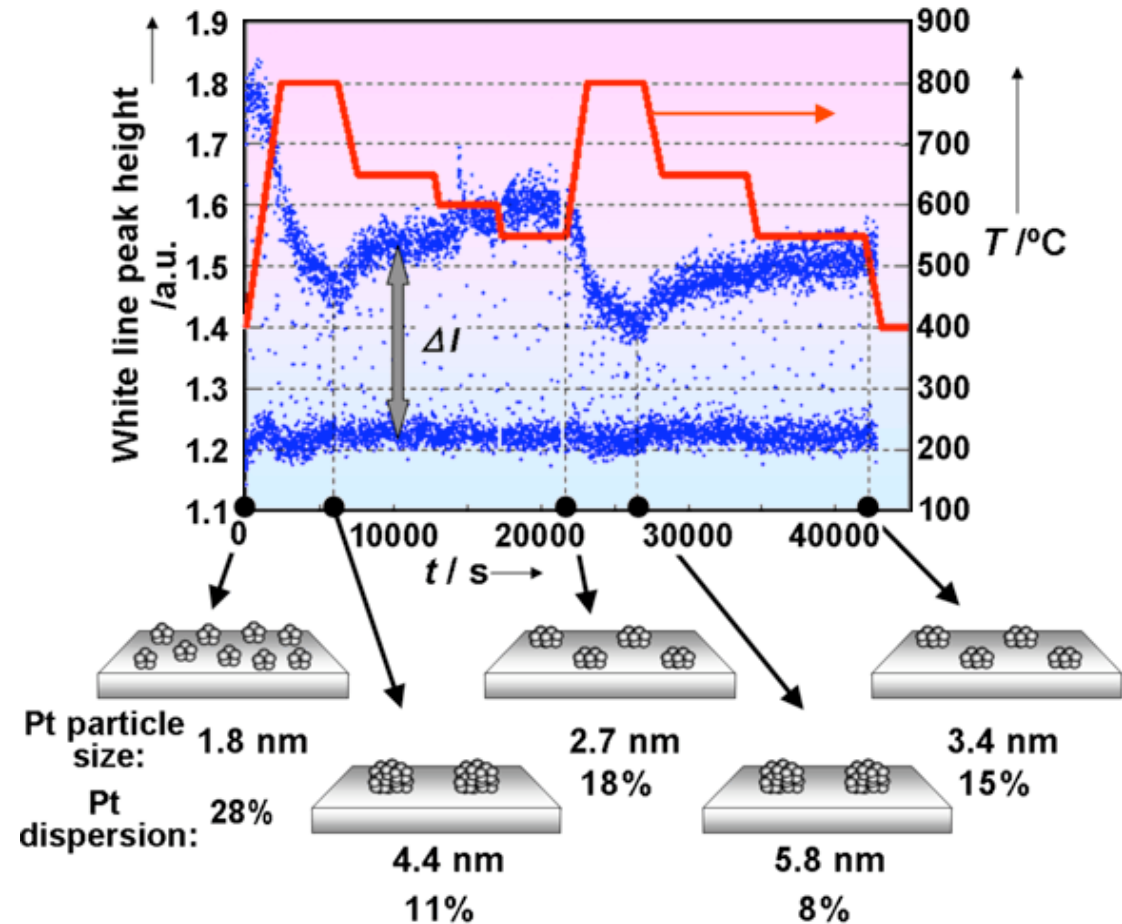
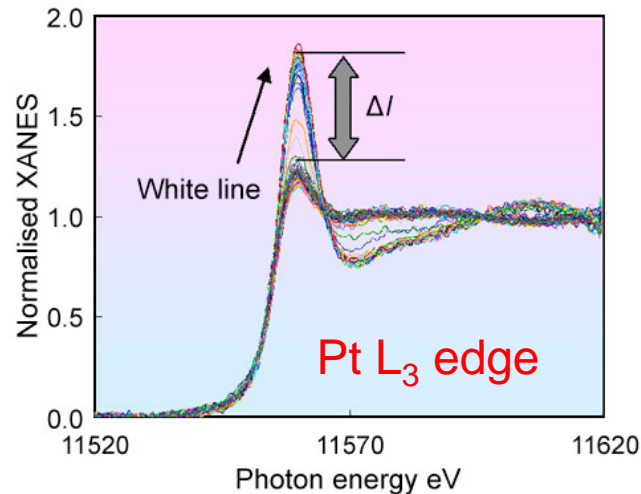
Bulk

$N=4$

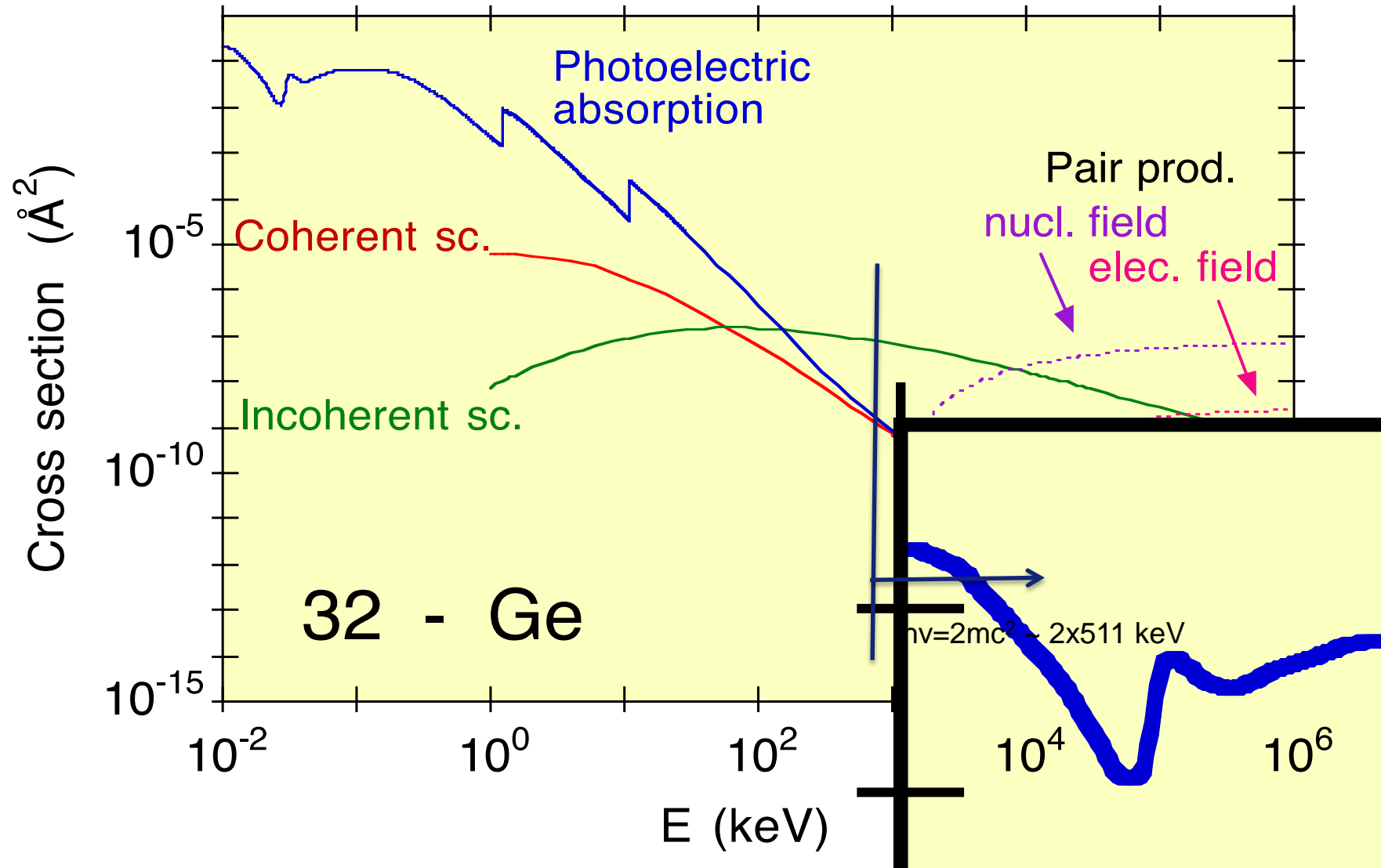
Complex EXAFS structure

TIME - RESOLVED XANES : CATALYSIS STUDIES

Time resolved absorption spectroscopy could help in understanding the mechanism of CO catalysis at interfaces by monitoring the time evolution of oxidation state of Pt.



SCATTERING AND ABSORPTION CROSS SECTIONS



POLARIZATION DEPENDENT ABSORPTION

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

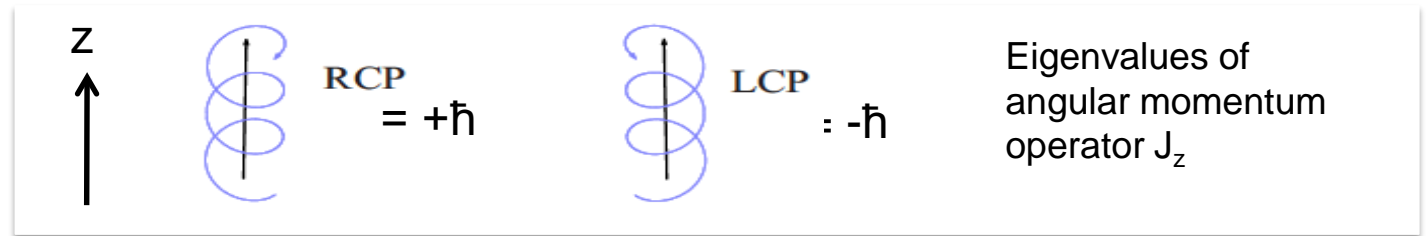


Combination of $\lambda/4$ and linear polarized filters have the different effect on circular polarization. Circular dichroism is found also in chiral molecules which select only one circular polarization (ex. sugar)

X-RAYS MAGNETIC CIRCULAR DICHROISM

Quantum description of a circular polarised photon beam:

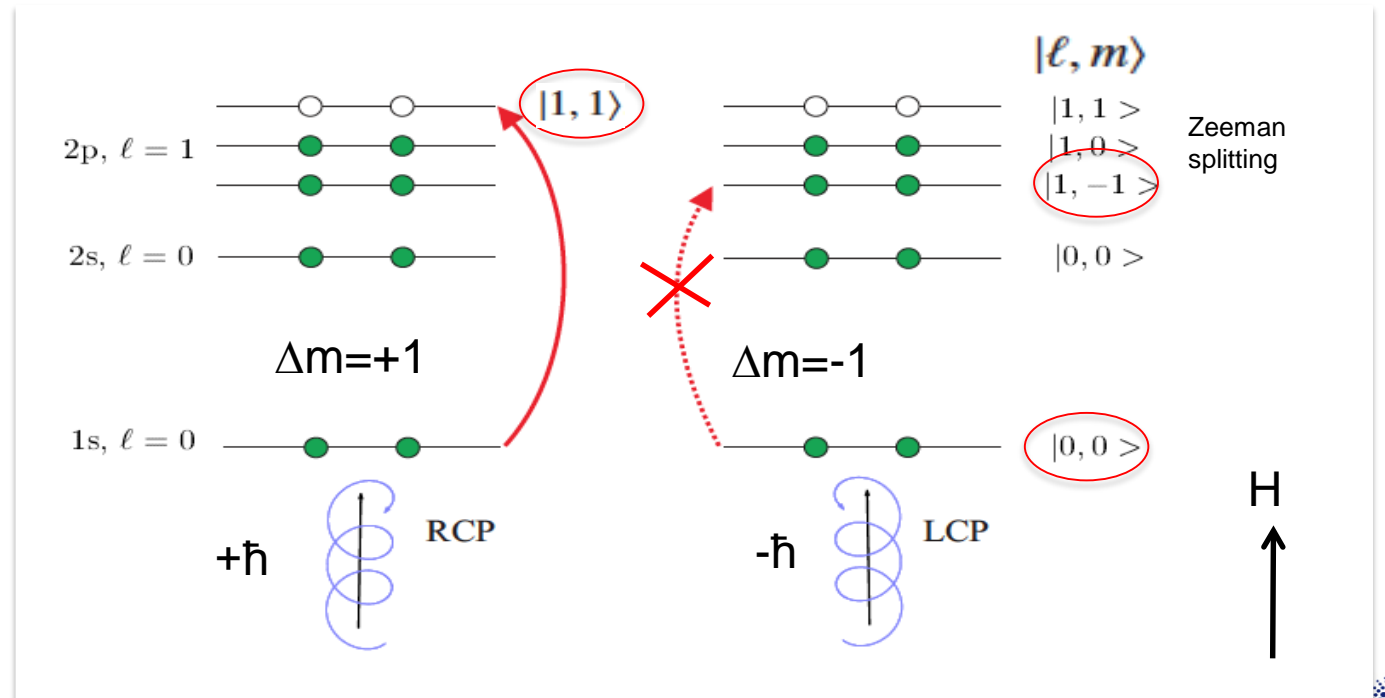
RCP and LCP eigenstates of J_z



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 (E1)
 selection rule: $\Delta l \pm 1$
 (odd function for coordinate exch.)

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

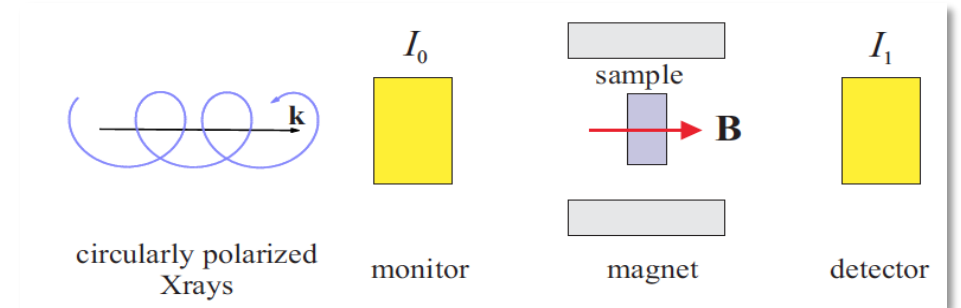


X-RAY MAGNETIC CIRCULAR DICHOISM

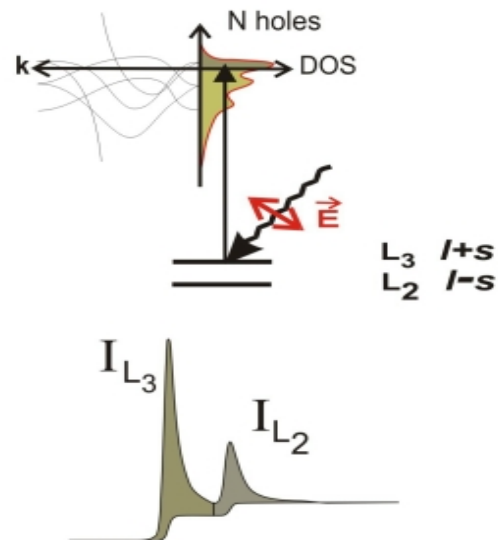
X-ray magnetic dichroism is the difference in the absorption coefficients μ^\pm of left (-) and right (+) circularly polarized x-rays.

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

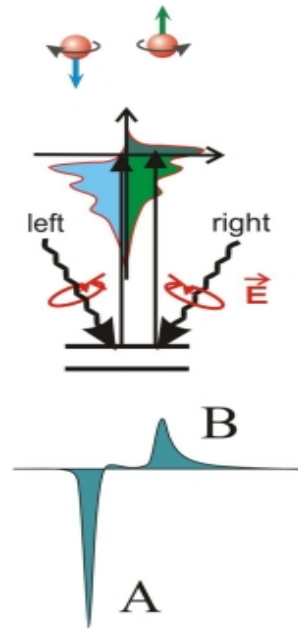
$$\mu^-(E) = \left(\frac{1}{d}\right) \ln \left(\frac{I_0^-(E)}{I_1^-(E)}\right)$$



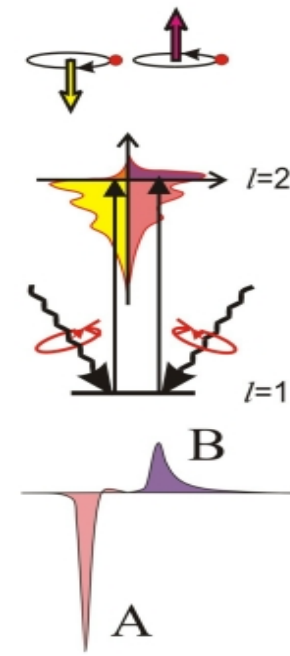
Orbital occupation
(linear dichroism)



Spin moment



Orbital moment



SINGLE MOLECULE MAGNETS ON FERROMAGNETIC METALS

A. Lodi Rizzini et al., *Phys. Rev. Lett.* 107, 177205 (2011)

Single molecule magnets are ideal candidates for magnetic data storage and quantum computing applications.

Element-resolved magnetization measurements using X-ray magnetic circular dichroism (soft x-rays)

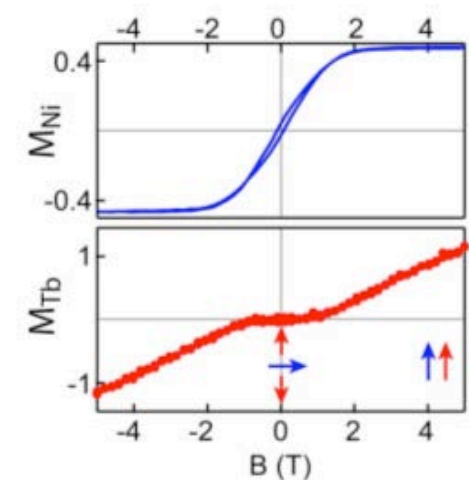
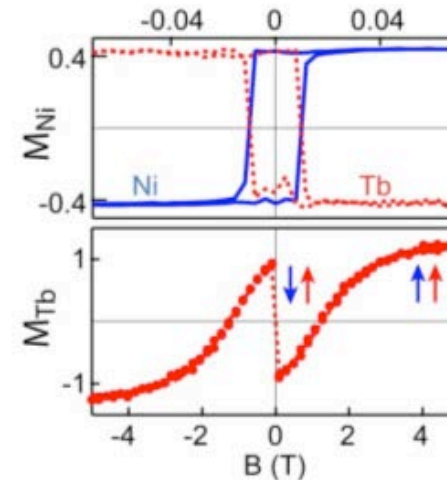
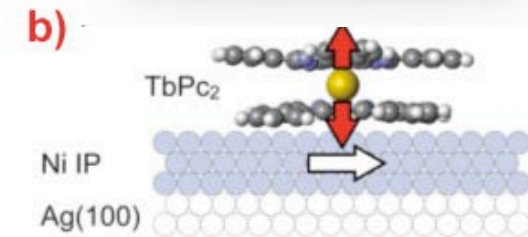
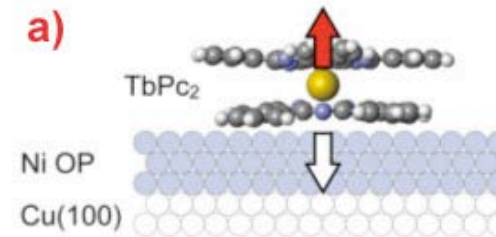
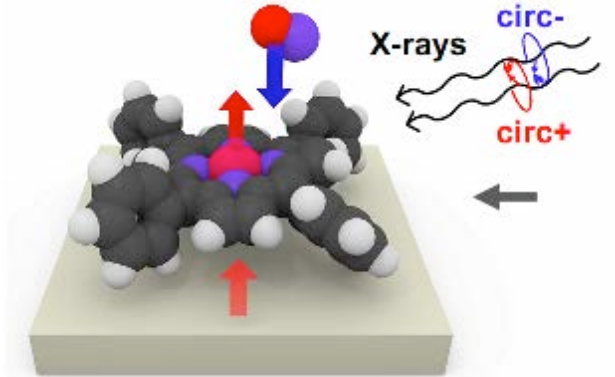
Tb-complex on Ni metal film

- a) Cu(110) substrate -> out-of-plane magnetization
- b) Ag(100) substrate -> in-plane magnetization

a) Ni AF to Tb at H=0

H-dependent F or AF coupling
finite remanent magn. up to 100K
square hysteresis loop

b) Frustrated Tb magnetization
zero remanence at H=0



X-rays optical properties

SCATTERING AND REFRACTION INDEX

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

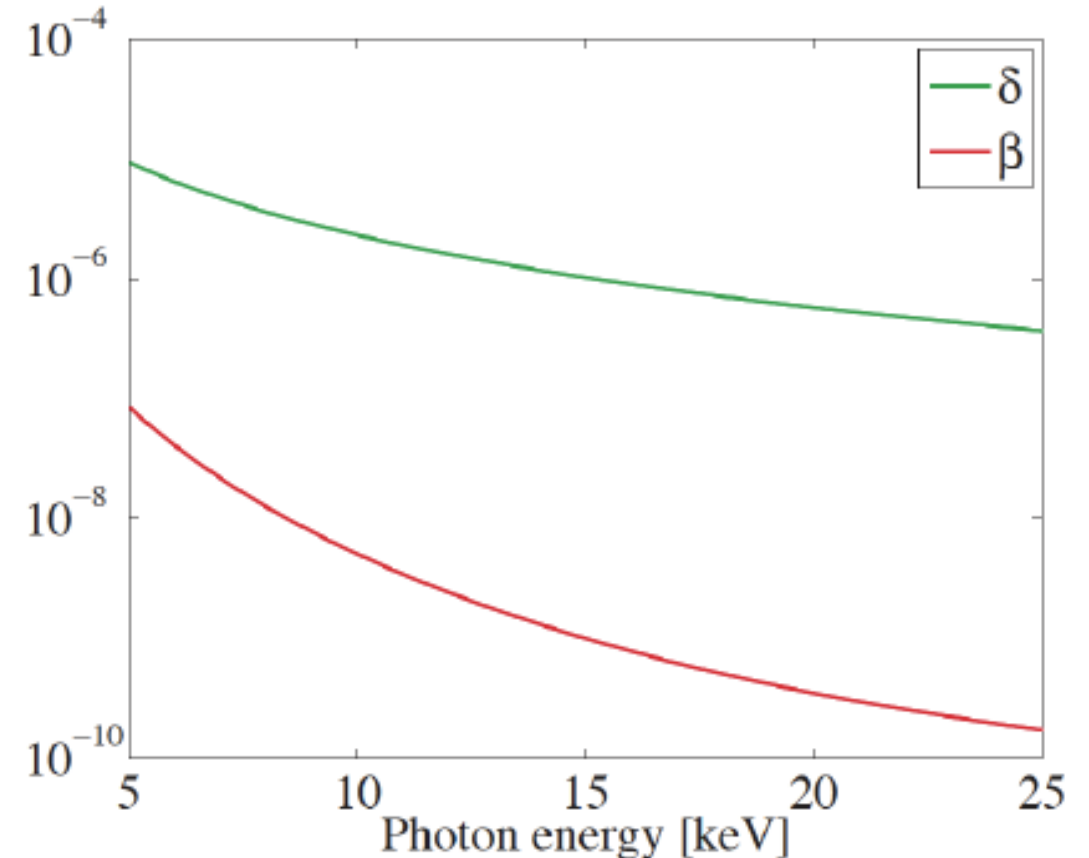
The existence of resonant scattering terms arising from the dispersion corrections can therefore be expected to lead to a frequency dependence of the refractive index n .

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

$$\delta = (f^0(Q) + f') \frac{2\pi\rho_{at}r_0}{k^2}$$

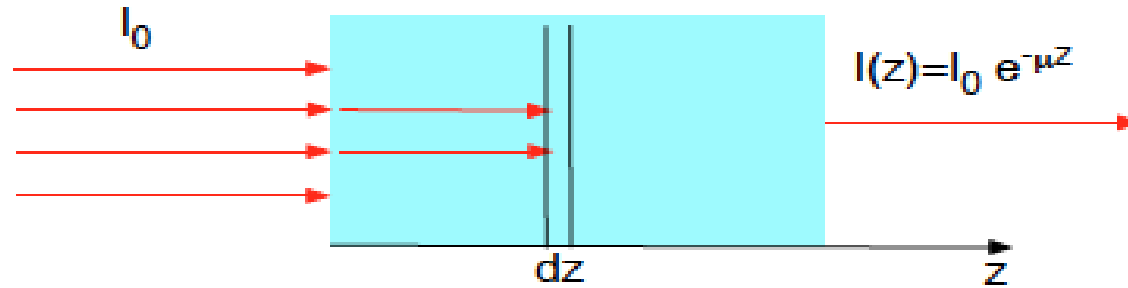
$$\beta = -f'' \frac{2\pi\rho_{at}r_0}{k^2}$$

$$\rho_{at} = \sum_i \frac{Z_i}{V_m} \quad \text{atomic number density}$$



REFRACTIVE INDEX AND ABSORPTION COEFFICIENT μ

X-rays propagating from vacuum to an absorbing medium of thickness Z

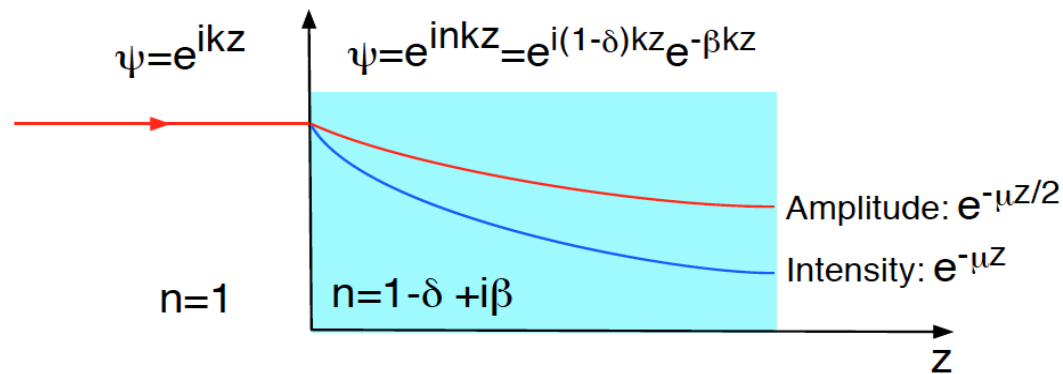


$I(z)$ attenuated transmitted wave

$\mu =$ absorption coefficient (m^{-1})

The attenuation length μ^{-1} is the distance where the intensity of the transmitted beam has dropped to $1/e$

The waves amplitude is attenuated (β) and phase shifted (δ)



Relation between the absorption and the refraction index

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

Taking into account the Thomson dispersion corrections

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

$$\delta = (f^0(0) + f') \frac{2\pi \rho_{at} r_0}{k^2}$$
$$\beta = -f'' \frac{2\pi \rho_{at} r_0}{k^2}$$

Forward direction $Q=0$

Relation between the imaginary part of anomalous dispersion and the absorption coefficient

$$f'' = - \left(\frac{k^2}{2\pi \rho_{at} r_0} \right) \frac{\mu}{2k}$$

And because $\mu = \rho_{at} \sigma_a$

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

REFRACTION: X-RAYS AND VISIBLE LIGHT

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

Refraction index for X-rays:

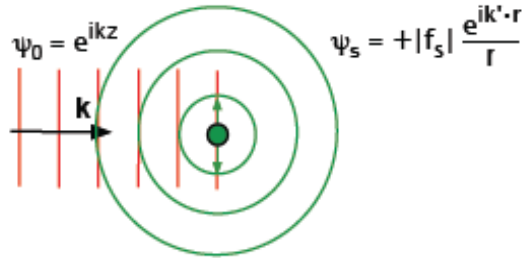
$$n = 1 - \delta + i\beta$$

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

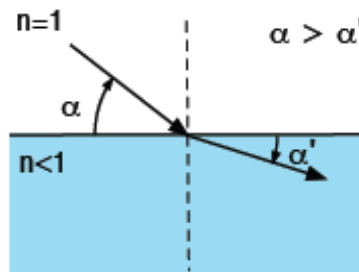
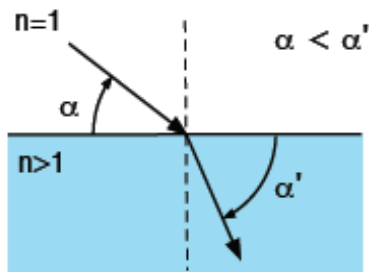
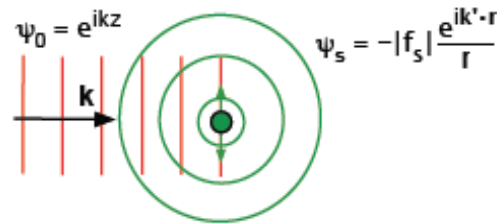
$$\delta(\text{solids}) \sim 10^{-5}$$

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

Visible light

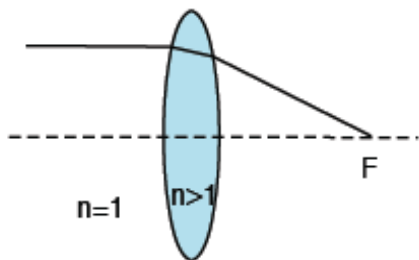


X-rays

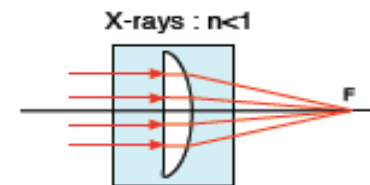
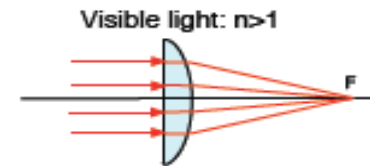
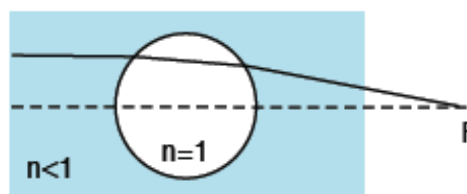


Low focusing power compared with the visible light

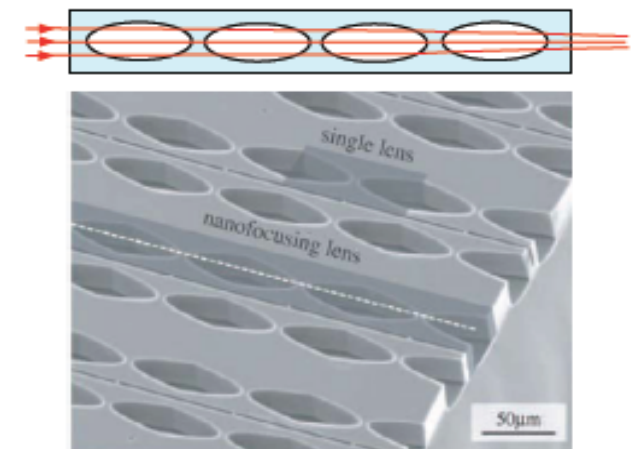
Optic lenses



X-rays lenses

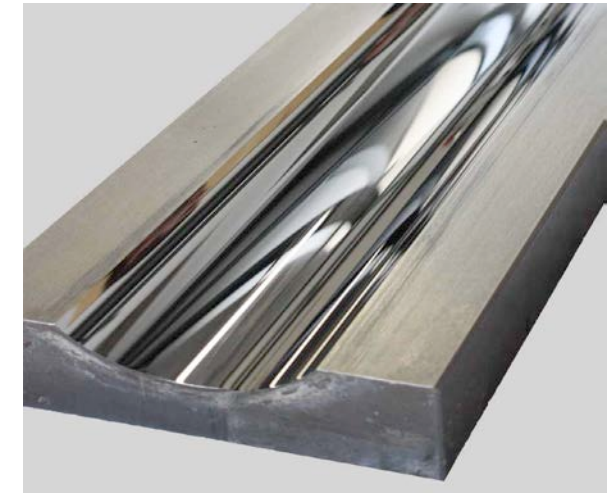
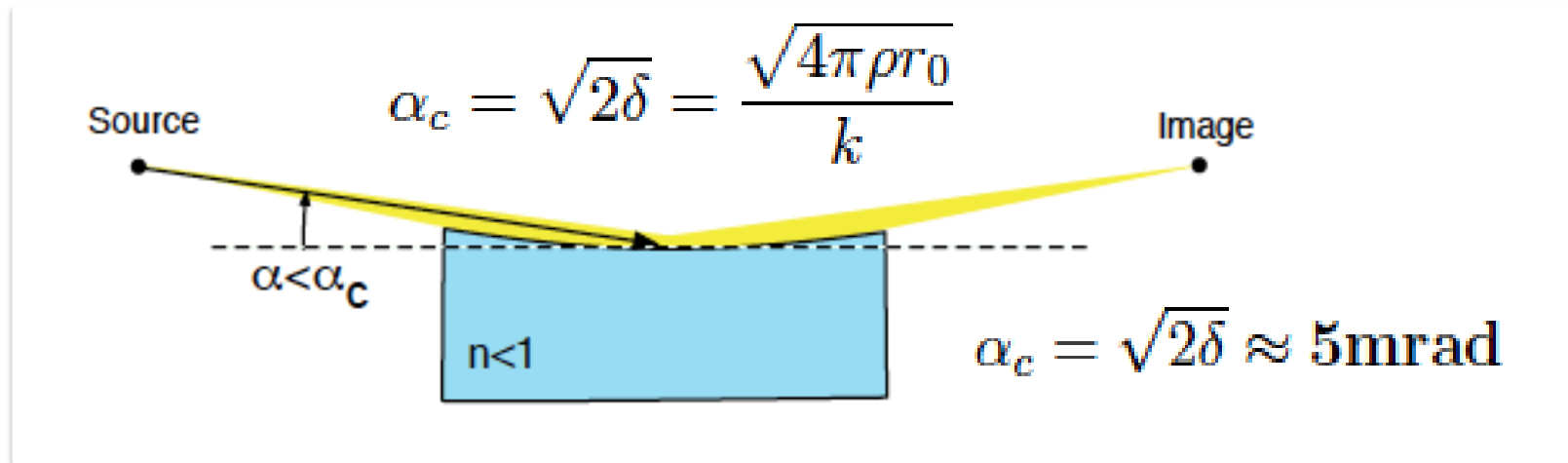


Compound refractive lenses for X-rays



X-RAY FOCUSING MIRRORS

The critical angle for the total reflection



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

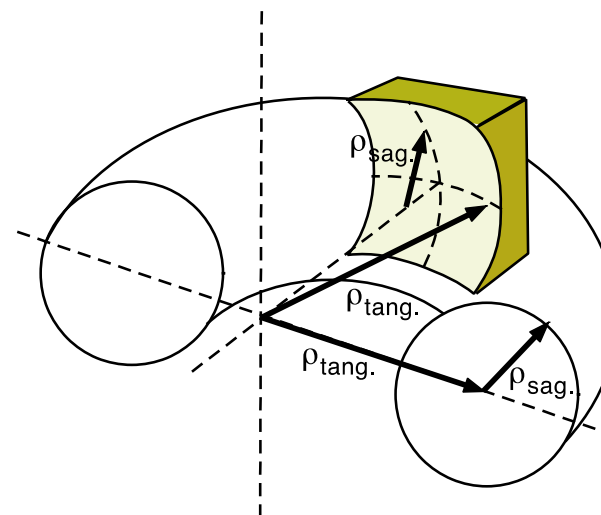
Ex: silicon mirror with toroidal shape

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

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

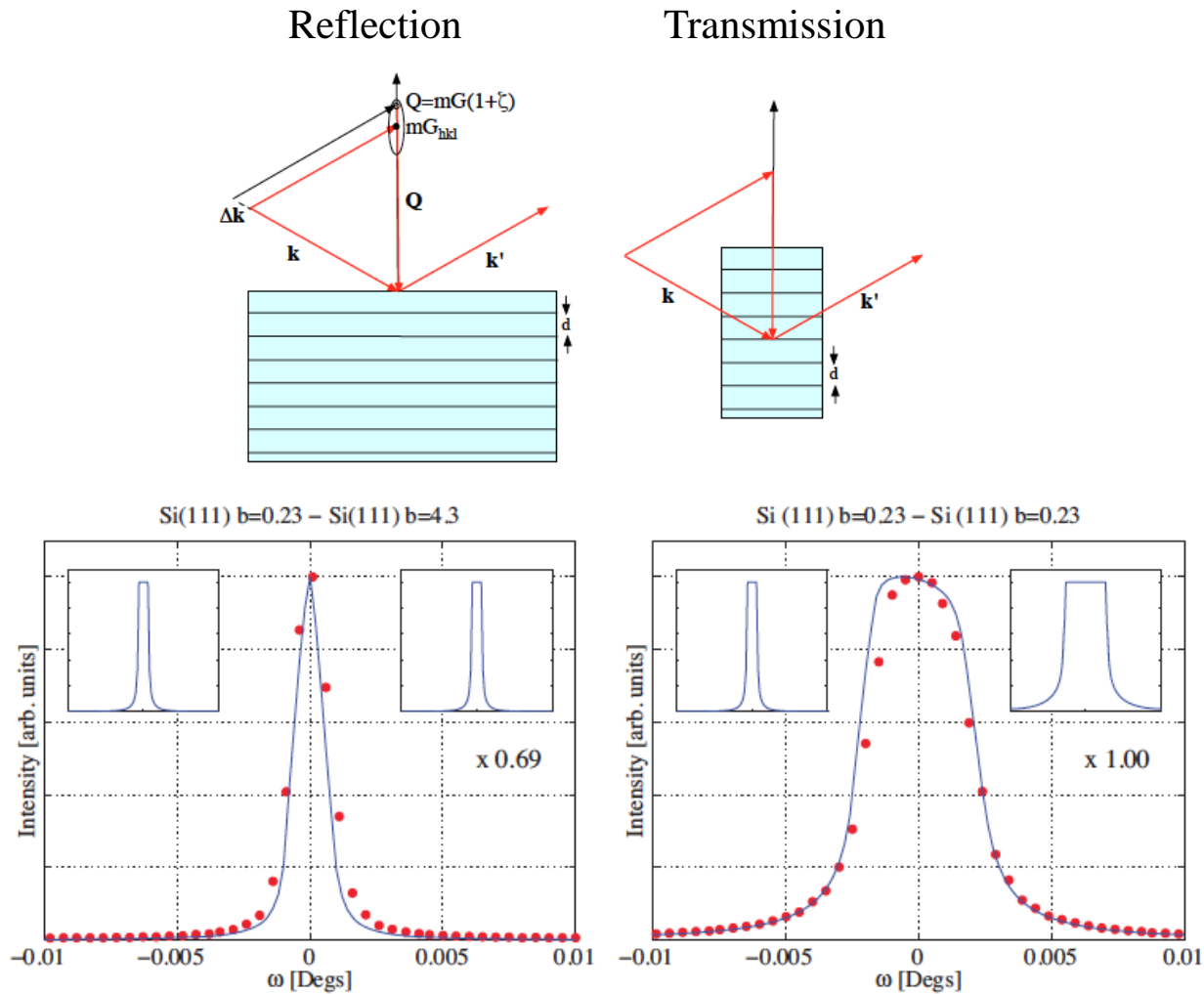
$\theta=2.7 \text{ mrad}$

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

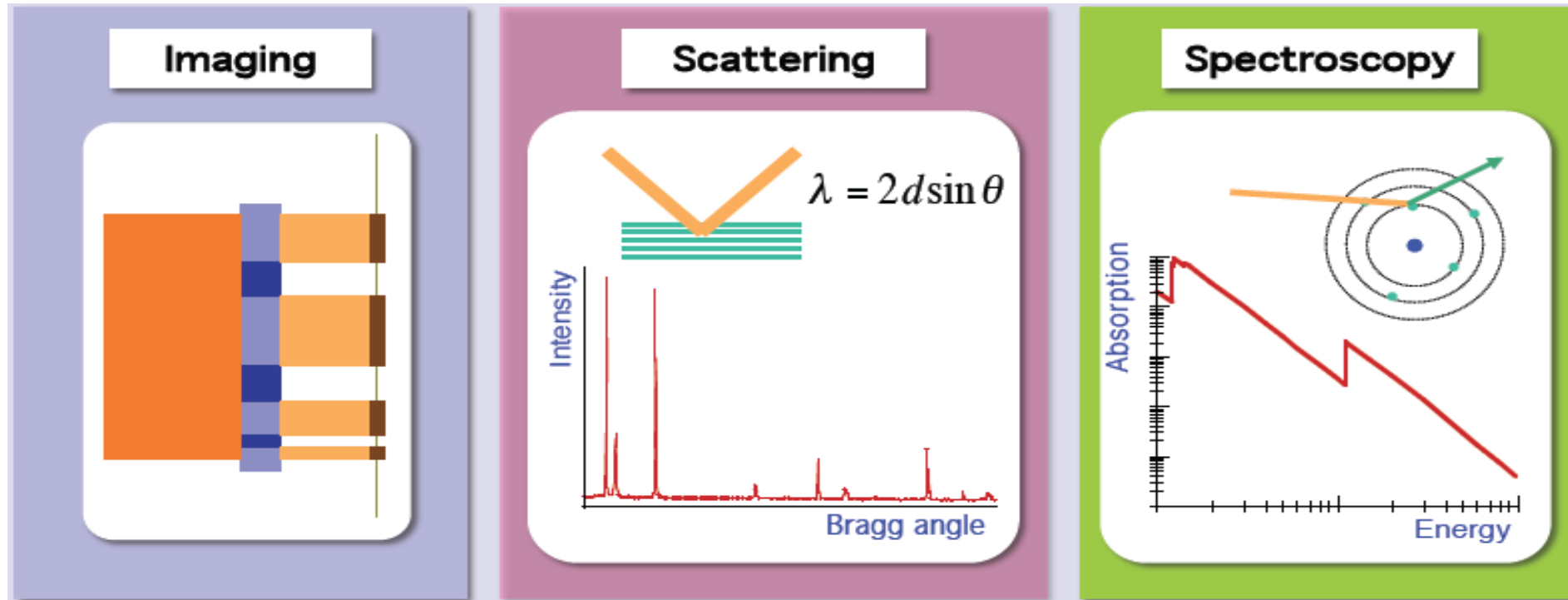


X-RAYS MONOCHROMATORS

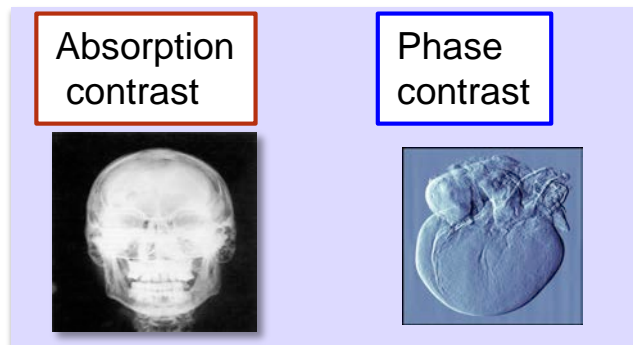
The Bragg diffraction from perfect crystals select a wavelength λ from the synchrotron radiation spectrum emitted by bending magnets or undulators



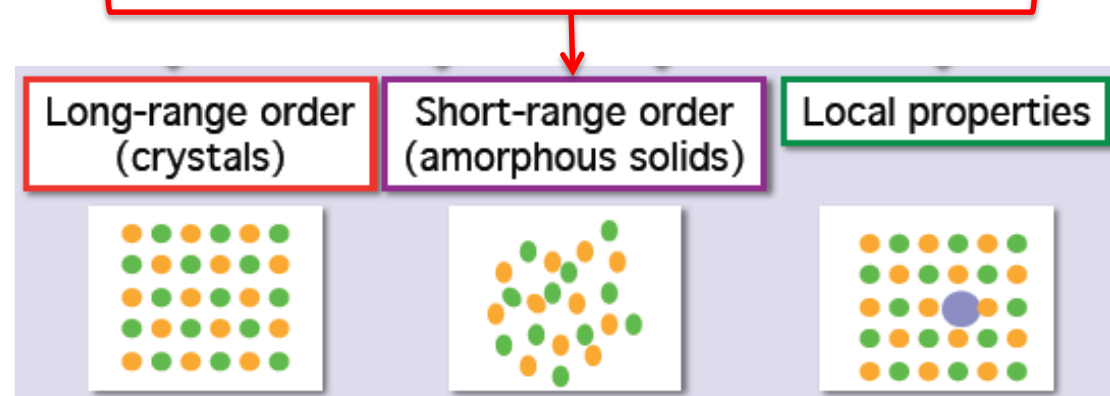
X-RAY SCATTERING METHODS



Spatial informations



Structural informations





Thank you for your attention!