Atoms, X-rays and Synchrotron Radiation

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Outline

- Light
- X-rays and Synchrotron radiation sources
  - X-rays and atoms
  - X-ray sources
- Detectors Basic Principles
  - Interactions of x-rays with matter
  - XAFS: EXAFS and XANES
- Gas Detectors
  - Ionization chambers
- Conclusions

INTERNATIONAL
YEAR OF LIGHT
2015

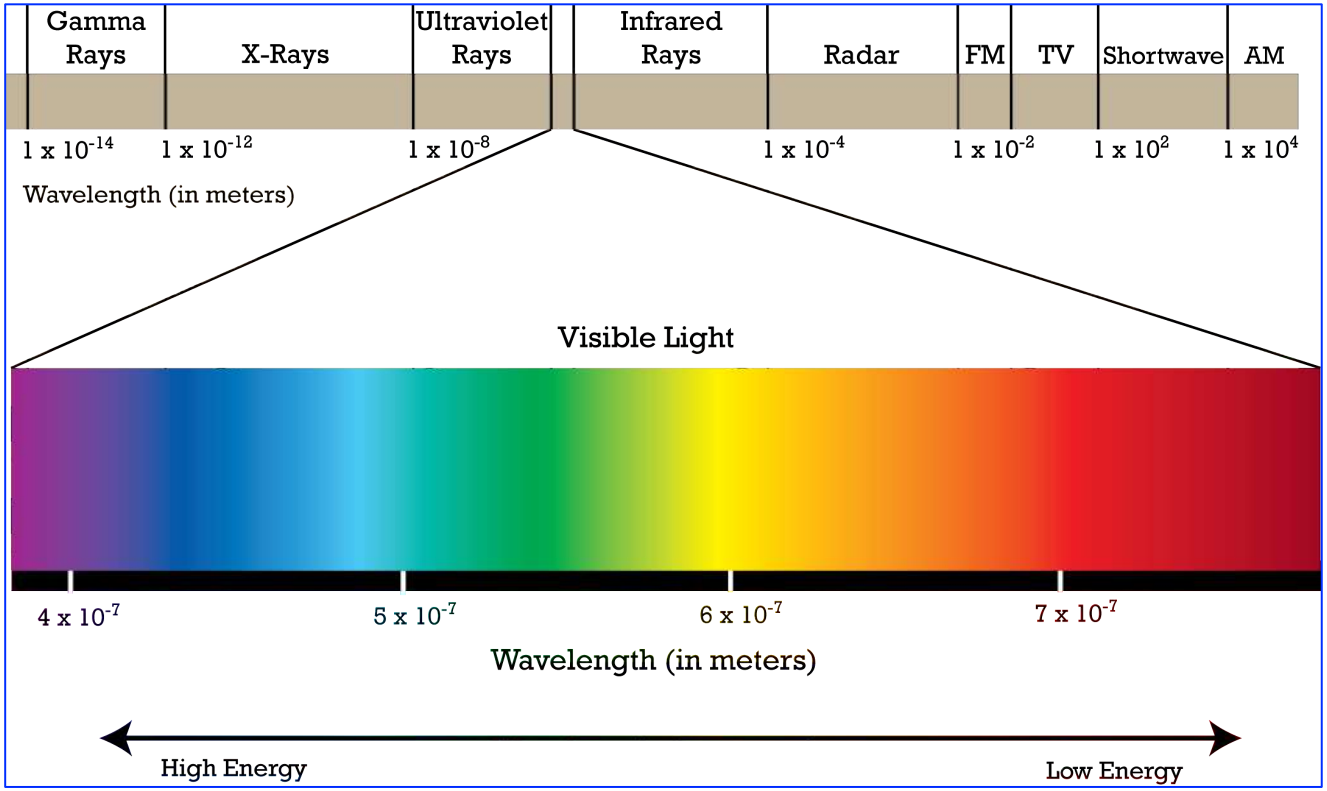
Light

Progress in science goes in parallel with the technical progress in producing and using light at different wavelengths to explore the physical world.

Light

Visible light is only a ***tiny slice of the electromagnetic spectrum***. The entire electromagnetic spectrum of light is huge, spanning from ***gamma rays on one end to radio waves***.

Visible Light is the light we can see using our eyes. This tiny human spectrum encompasses a very specific range of wavelengths from about ***380 nm to 780 nm***.

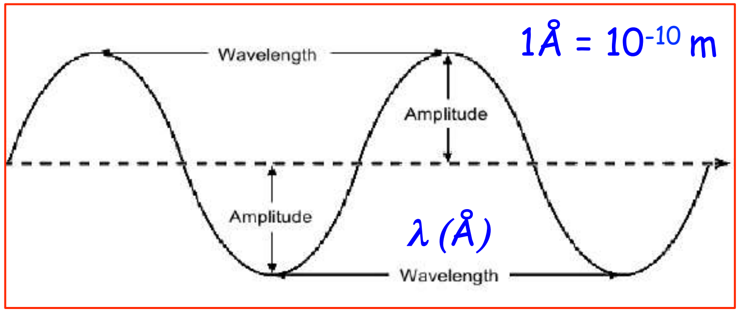


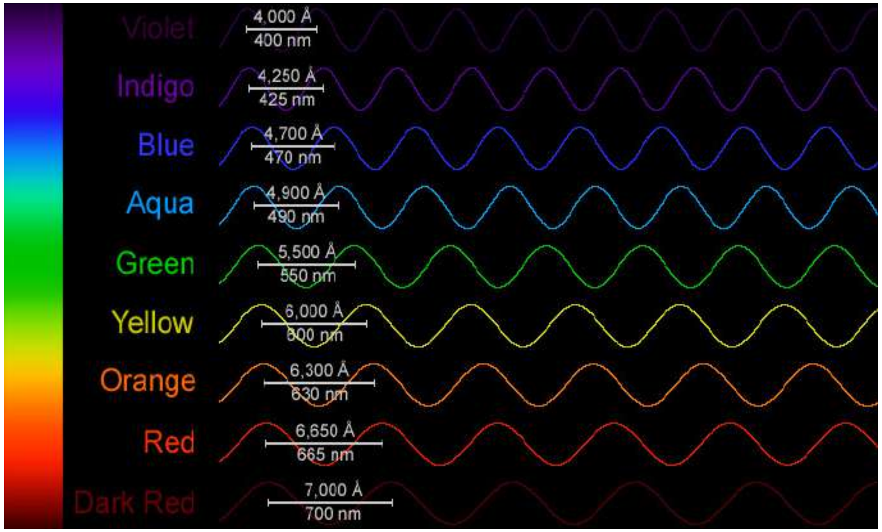
Physiologically we see these frequencies because the photoreceptors in our retinas are sensitive to them. When photons of light hit the photoreceptors this creates an electrochemical signal which is the first step in a fascinating process which ultimately results in us seeing colors.

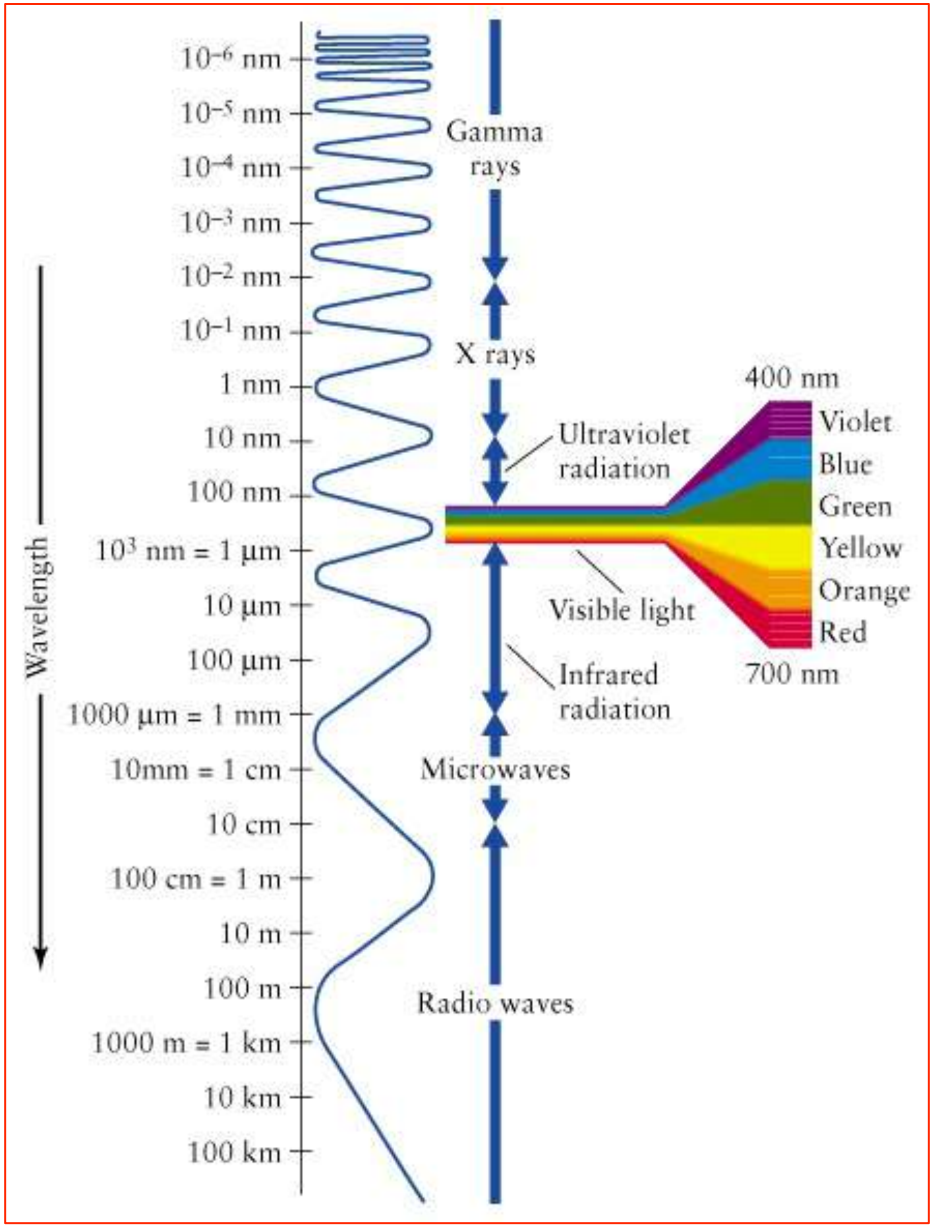
Light and waves

Light travels as waves of energy. Waves of light have different ***wavelengths*** (the distance between the top of one wave and the top of the next). ***Different colors of visible light have different wavelengths.***

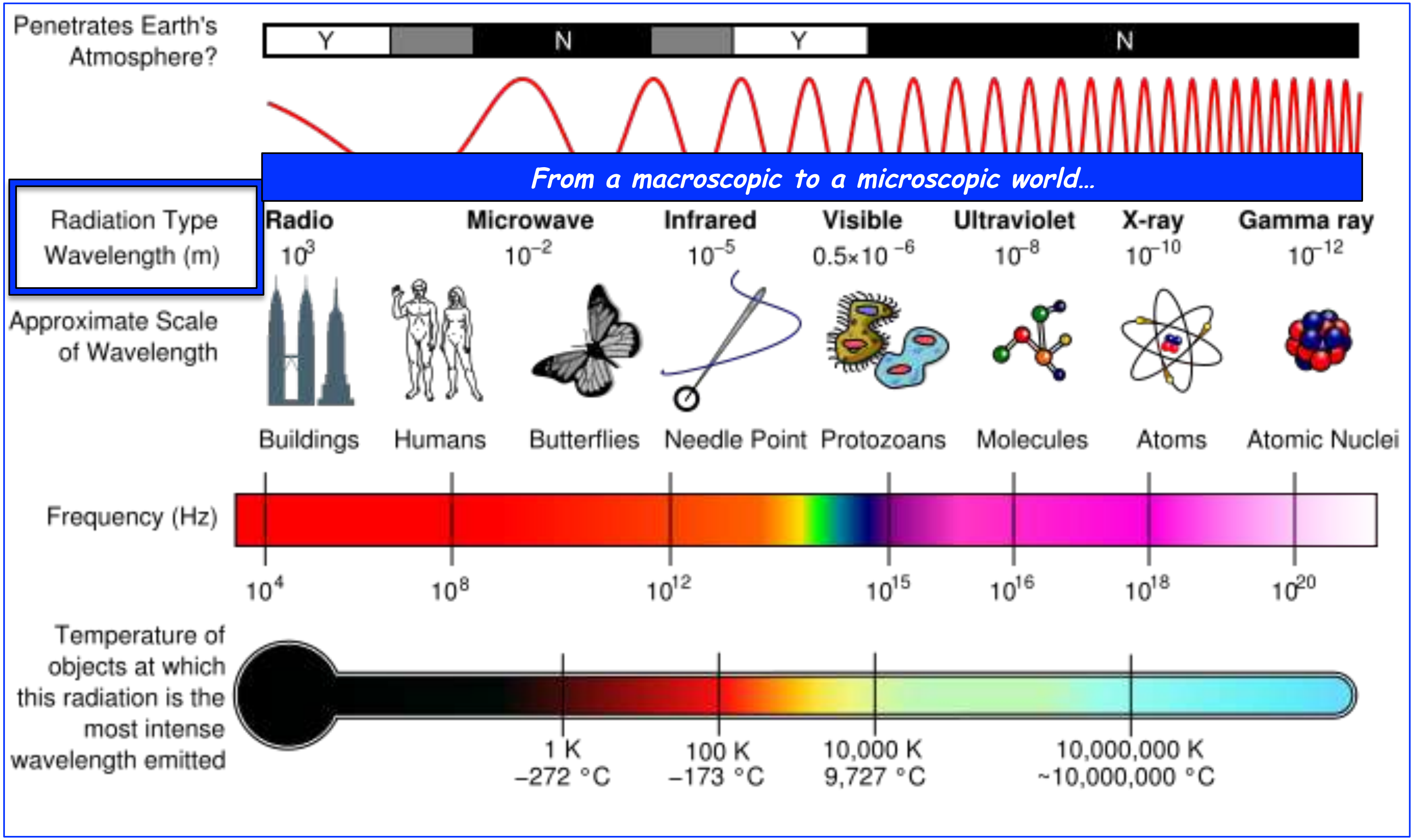
$1 Å = 10^{-10}$ m







Electromagnetic Spectrum



The ***wavelength*** (λ) and ***frequency*** (ν) ***of light are strictly related***: ***the higher the frequency the shorter the wavelength***! This is because ***all light waves move through vacuum at the same speed*** (*c* = speed of light) and the equation that relates wavelength and frequency for electromagnetic waves is: $\lambda\nu = c$

X-rays

X-rays discovery

EINE NEUE ART

VON

STRAHLEN.

VON

DR. W. RÖNTGEN,

O. Ö. PROFESSOR AN DER K. UNIVERSITÄT WÜRZBURG.

WÜRZBURG.

VERLAG UND DRUCK DER STAHEL'SCHEN K. HOF- UND UNIVERSITÄTS-BUCH- UND KUNSTHANDLUNG.

Ende 1895.

60 ₰.

On a New Kind of Rays

While ***Wilhelm Roentgen*** was working on the effects of ***cathode rays*** during ***1895***, he discovered X-rays. His experiments involved the passing of electric current through gases at extremely low pressure. On **November 8, 1895** he observed that certain rays were emitted during the passing of the current through discharge tube. His experiment that involved working in a totally dark room with a well covered discharge tube resulted in the **emission of rays which illuminated a barium platinocyanide screen**. ***The screen became fluorescent even though it was placed two meters away from discharge tube***.

Wilhelm Conrad Roentgen

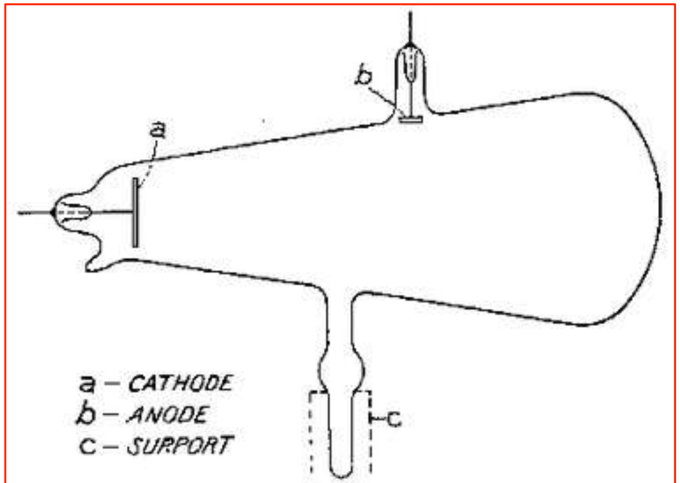
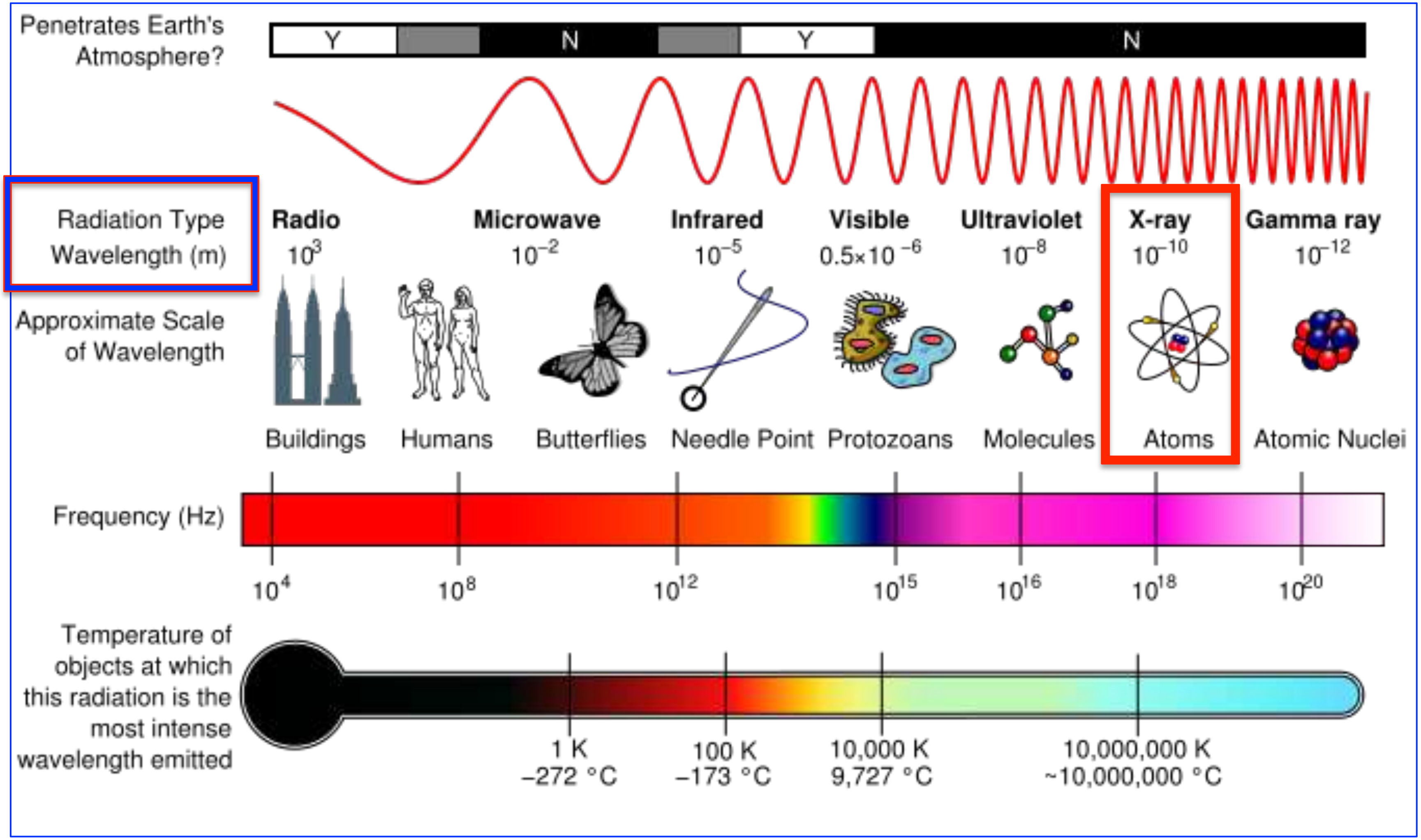


Fig. 1. Earliest type of roentgen tube.

Gas tube: electrons are freed from a **cold cathode by positive ion bombardment, thus necessitating a certain gas pressure.**

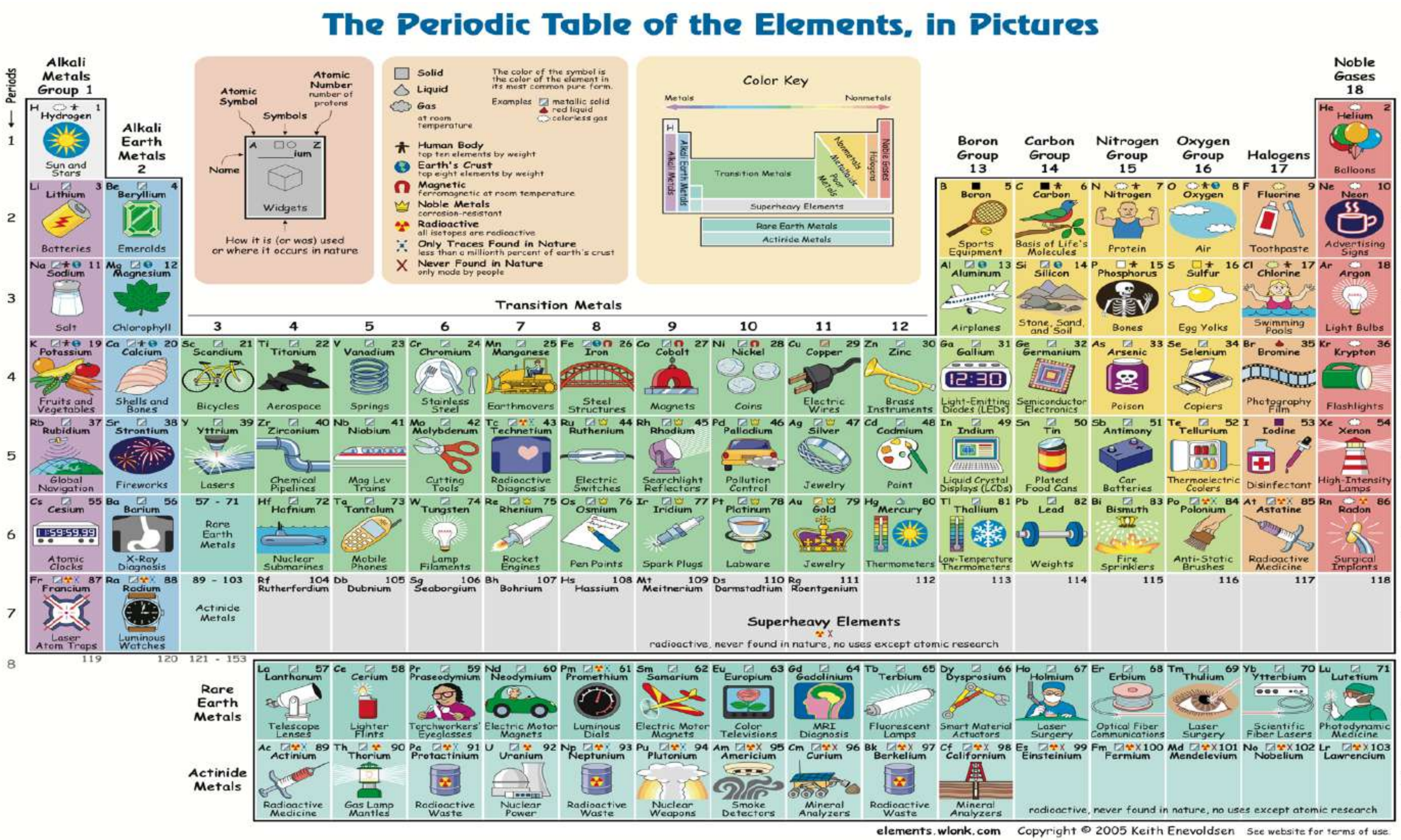
He continued his experiments using **photographic plates** and generated the very ***first "roentgenogram"*** by developing the image of ***his wife's hand*** and analyzed the variable transparency as showed by her bones, flesh and her wedding ring.

Electromagnetic Spectrum and X-rays

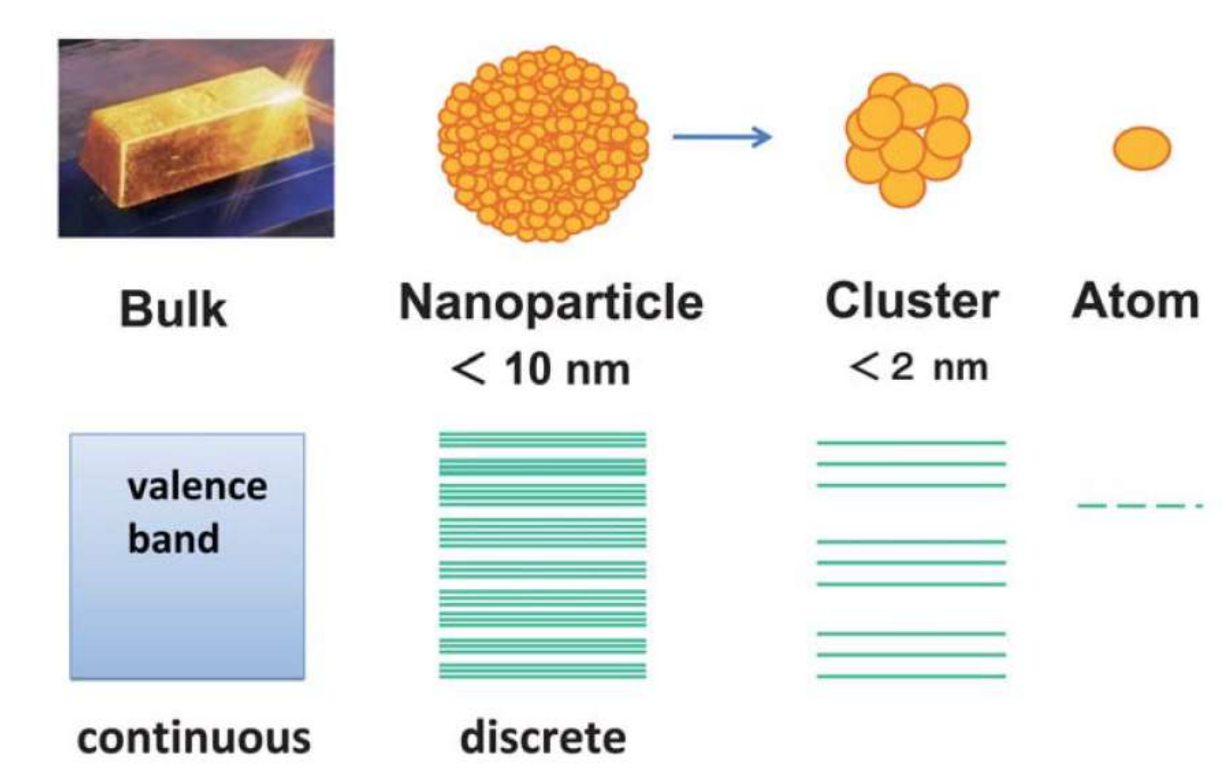


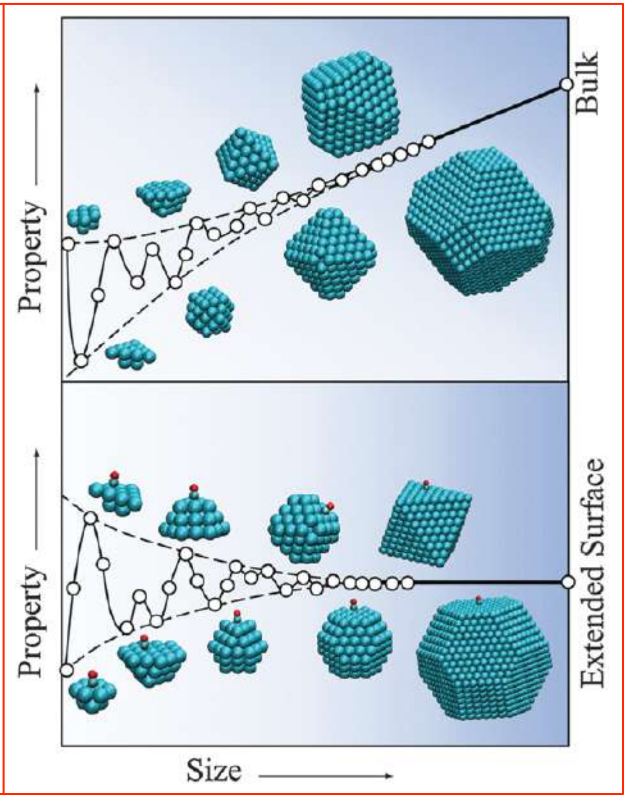
Atoms

Matter is everything around us! All matter such as solids, liquids, and gases, is composed of atoms. Therefore, atoms are considered to be the basic building block of matter. From the periodic table, it can be seen that there are only about 100 different kinds of atoms. These same 100 atoms form thousands of different substances ranging from the air we breathe to the metal used to support tall buildings.



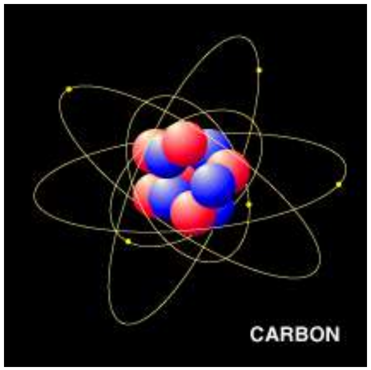
Atoms and physical properties





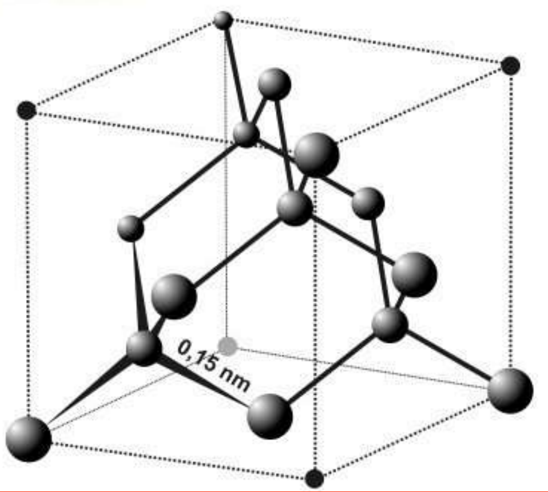
Gold coins and ingots have been highly prized for millennia. But scientists have realized that nanoparticles of this metal could have also quite important properties. In labs around the world, gold nanoparticles are being tested as components in technology and medicines. ***Gold nanoparticles could be used to kill cancer cells, improve the efficiency of solar cells and catalyze chemical reactions.***

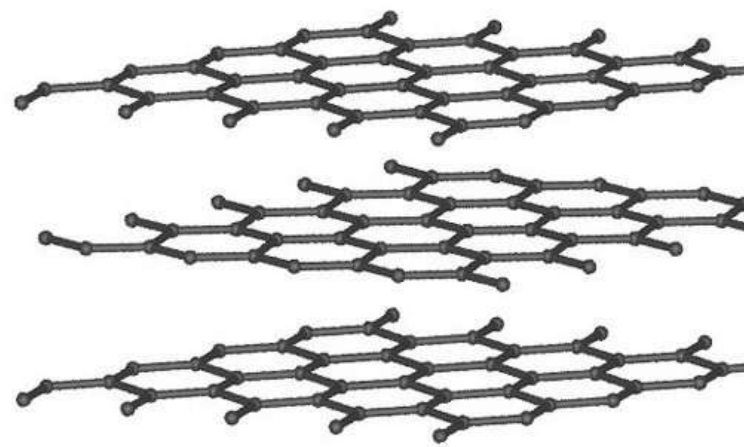
X-rays and Atoms



Both diamond and graphite are made entirely out of carbon!

Using x-rays to reveal the atomic structure of materials

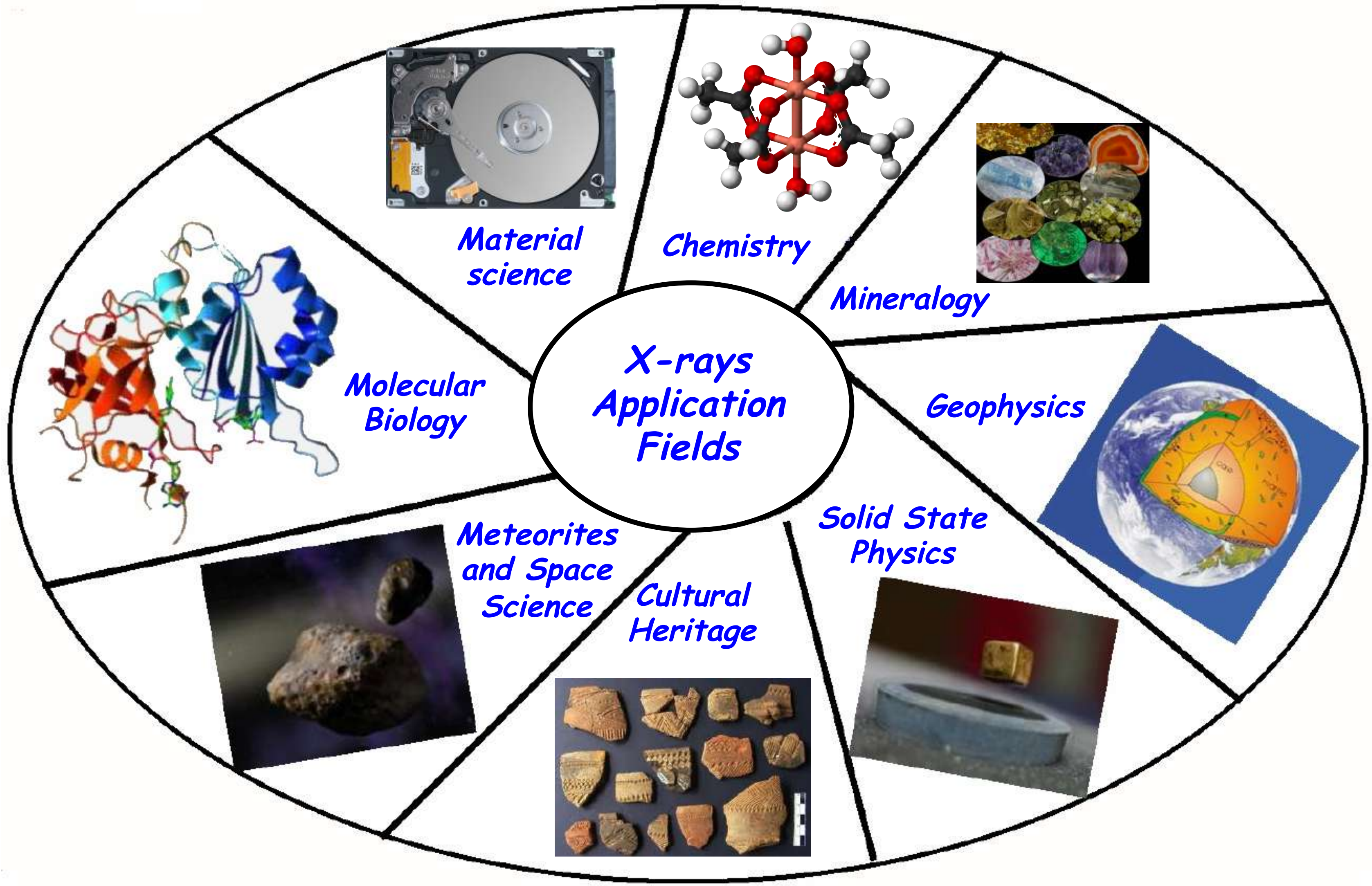




Graphite is opaque and metallic- to earthy-looking, while diamonds are transparent and brilliant.

The different properties of graphite and diamond arise from their distinct crystal structures.

X-rays application fields



Synchrotron radiation sources

Light sources

Fire *is not a very useful light source to see small details because its emitted power is* ***spread in all directions****!*

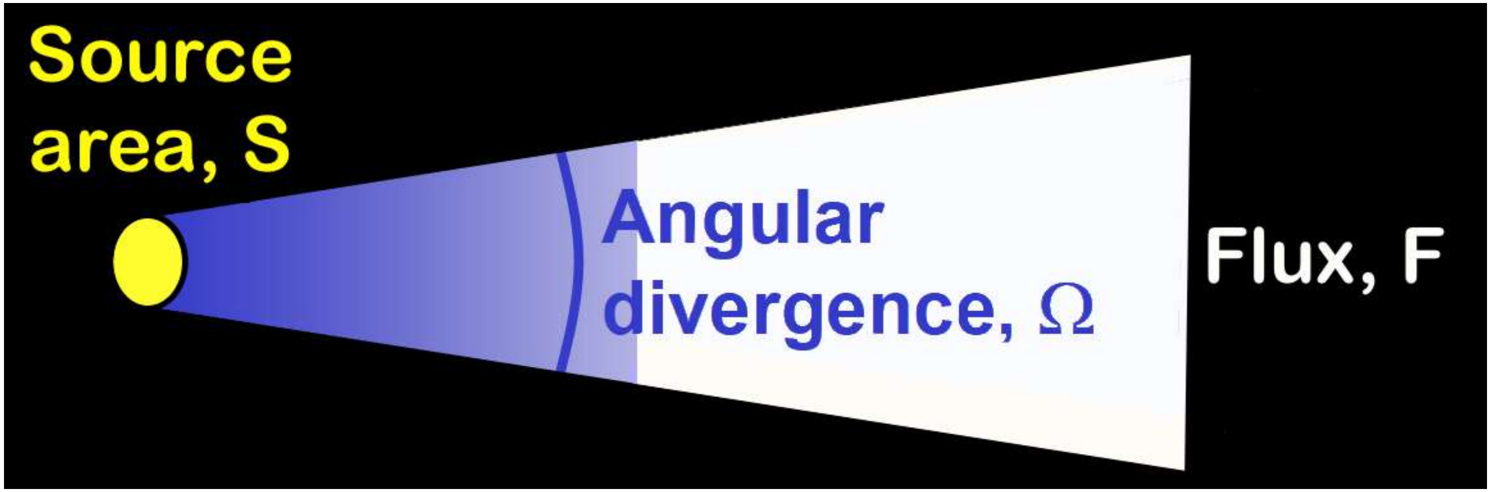
A torchlight is more adequate because due to its small size the emission is ***concentrated within a narrow angular spread: this a "bright" source****!*

Synchrotron radiation is a very bright light source *that, as will be shown, gives us the chance to* ***study also things that we cannot "see " with our eyes using not visible light but X-rays****!*

Light sources and brightness

When interested in nm scale details: brightness becomes fundamental.

A ***bright source*** is the one ***very effective in illuminating a specific target***. If the specific target is small a ***bright source*** is ***a small size source with emission concentrated within a narrow angular spread.***



$$\text{Brightness} = \text{constant}\ \frac{F}{S \times \Omega}$$

Bright X-ray sources?

HE particle accelerators

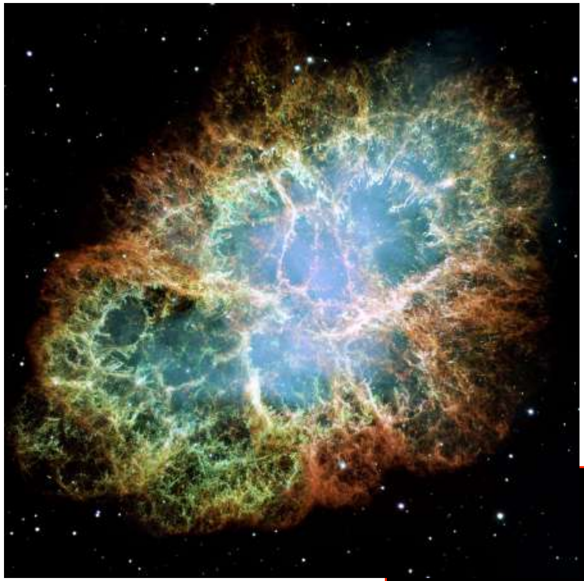
↓

Relativistic effects

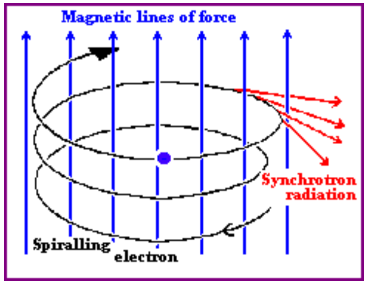
↓

Synchrotron light

Synchrotron light is present in nature!



NASA Hubble Space Telescope image of the Crab Nebula (NASA, ESA and Allison Loll/Jeff Hester (Arizona State University)).



NASA's Great Observatories' View of the Crab Nebula X-Ray-blue: NASA/CXC/J.Hester (ASU); Optical-red and yellow: NASA/ESA/J.Hester & A.Loll (ASU); Infrared-purple: NASA/JPL-Caltech/R.Gehrz (Univ. Minn.)

Synchrotron radiation is a very important emission process in astrophysics!

Crab Nebula: remnant of a supernova explosion seen on earth by Chinese astronomers in 1054, at about 6500 light years from Earth in the constellation Taurus !

SR emission is produced by high energy electrons whirling around the magnetic fields lines originating from a Pulsar

The heart of the nebula is a rapidly-spinning neutron star, a pulsar, that powers the strongly polarised bluish 'synchrotron' nebula.

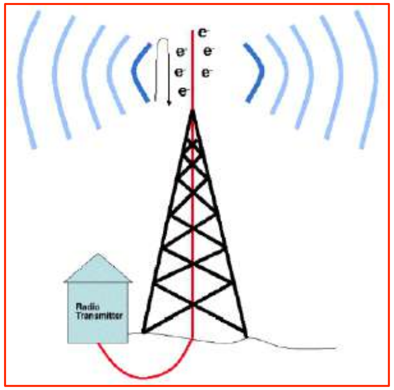
The ***Crab pulsar*** is ***slowing at the rate of about 10^{-8} sec per day***, and the ***corresponding energy loss agrees well with the energy needed to keep the nebula luminous***. Some of this luminosity takes the form of ***synchrotron radiation, requiring a source of energy for accelerating charged particles***.

*Composite image data from **three of NASA's Great Observatories**. The **Chandra X-ray Observatory image** is shown in blue, the **Hubble Space Telescope optical image** is in red and yellow, and the **Spitzer Space Telescope's infrared** image is in purple. The X-ray image is smaller than the others because extremely energetic electrons emitting X-rays radiate away their energy more quickly than the lower-energy electrons emitting optical and infrared light. **The Crab Nebula is one of the most studied objects in the sky, truly making it a cosmic icon**.*

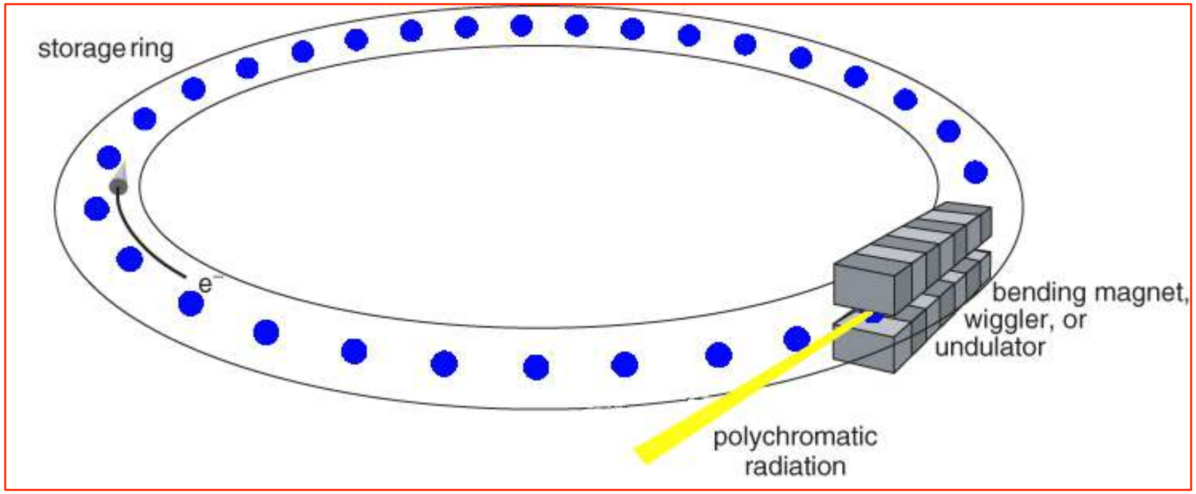
Synchrotron radiation

Accelerated NON relativistic charged particle, e^+, e^- and ions, emit electromagnetic radiation like electric charges forced to oscillate along an antenna.

$v \ll c$ or $\beta = v/c \ll 1$

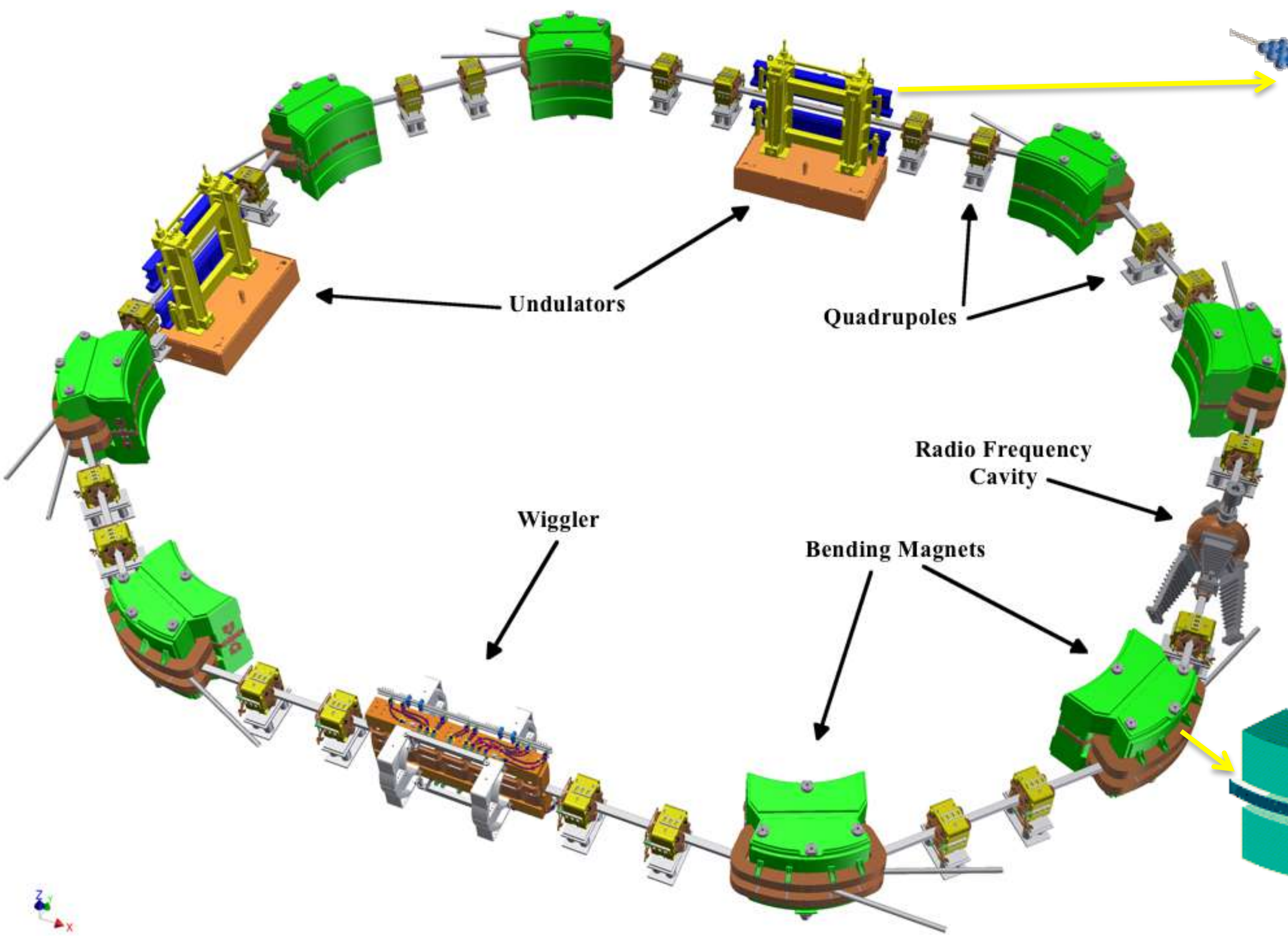


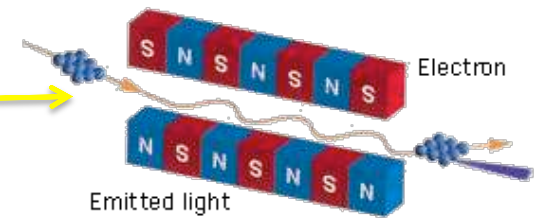
*When **charged particles, moving at RELATIVISTIC speeds** ($v \approx c$), are forced to **change the direction of their motion (acceleration)**, under the effect of **magnetic fields**, in **circular particle accelerators, like synchrotrons**, the radiation produced is called **Synchrotron Radiation**.*



$v \approx c$ or $\beta = v/c \approx 1$

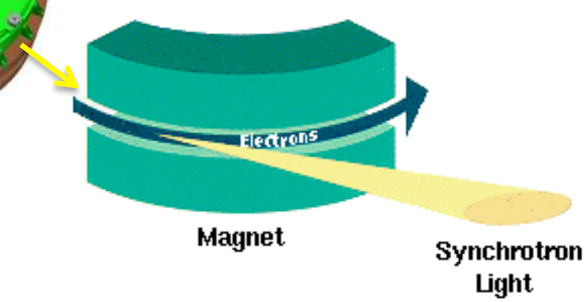
Synchrotron light is artificially produced by relativistic particles accelerated in circular orbits.





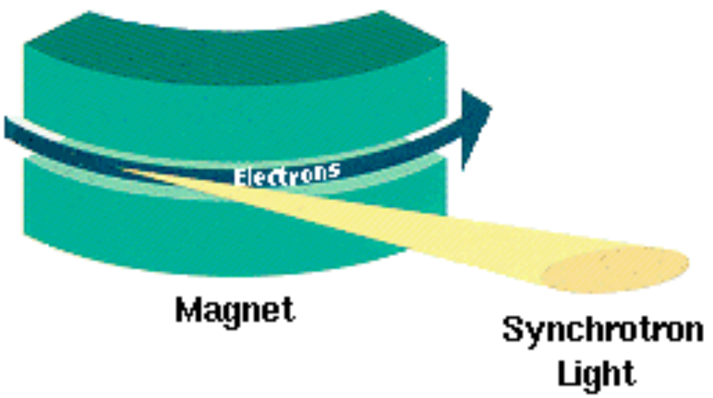
Insertion Device

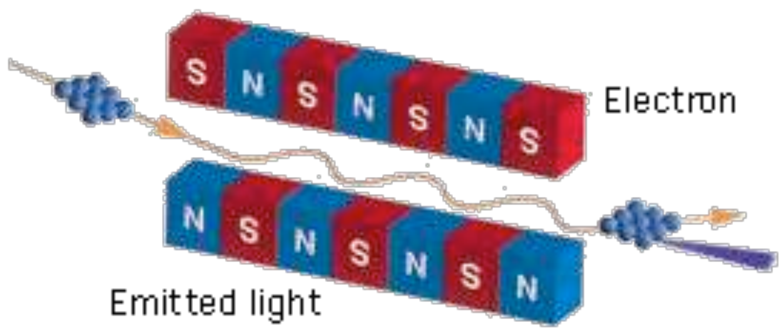
Bending Magnet



… and synchrotron radiation is also the coherent radiation emitted by the undulators of Free Electron Lasers.

Radiation sources



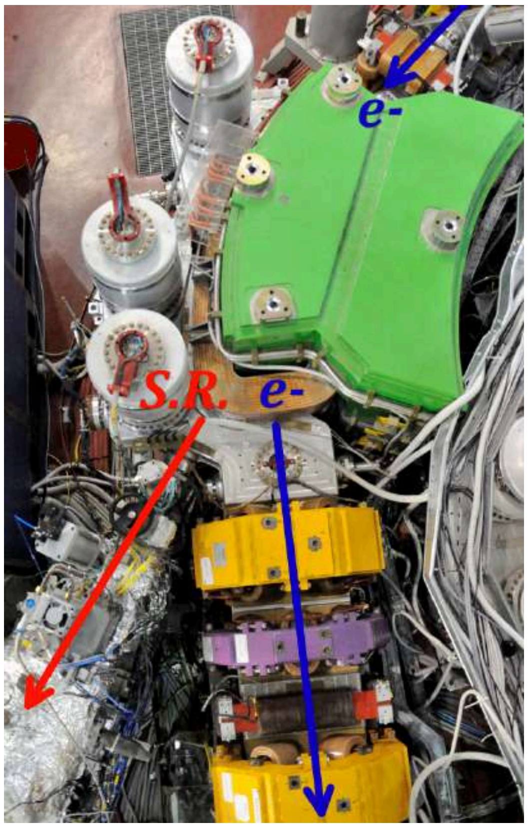


Bending magnet

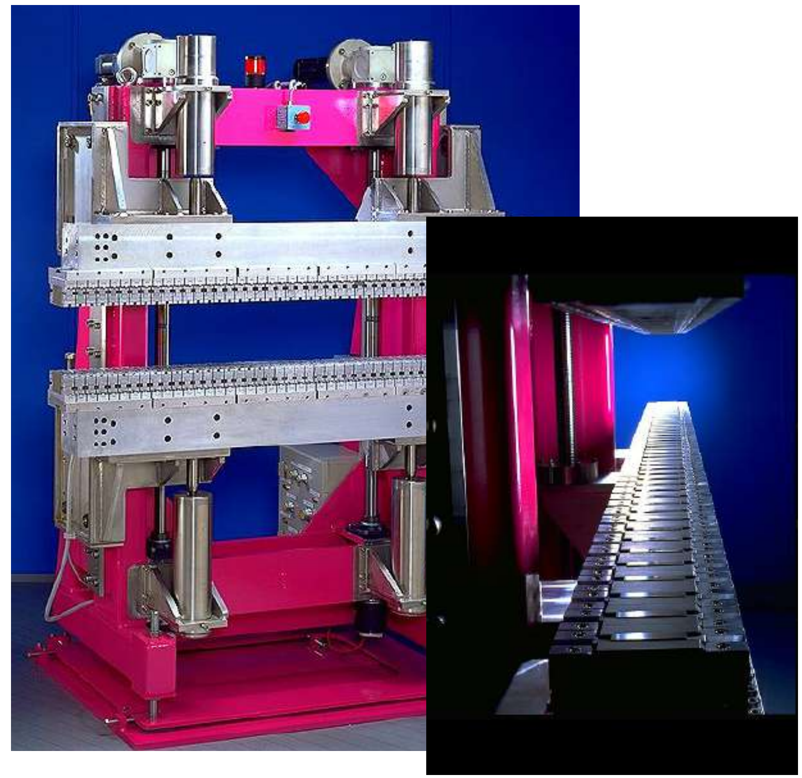
Undulator

Radiation Sources

There are two different sources of radiation in a storage ring:
- bending magnets (BMs)
- insertion devices (IDs) or periodic arrays of magnets inserted between the BMs (wigglers and undulators)



DAΦNE bending magnet (BM)

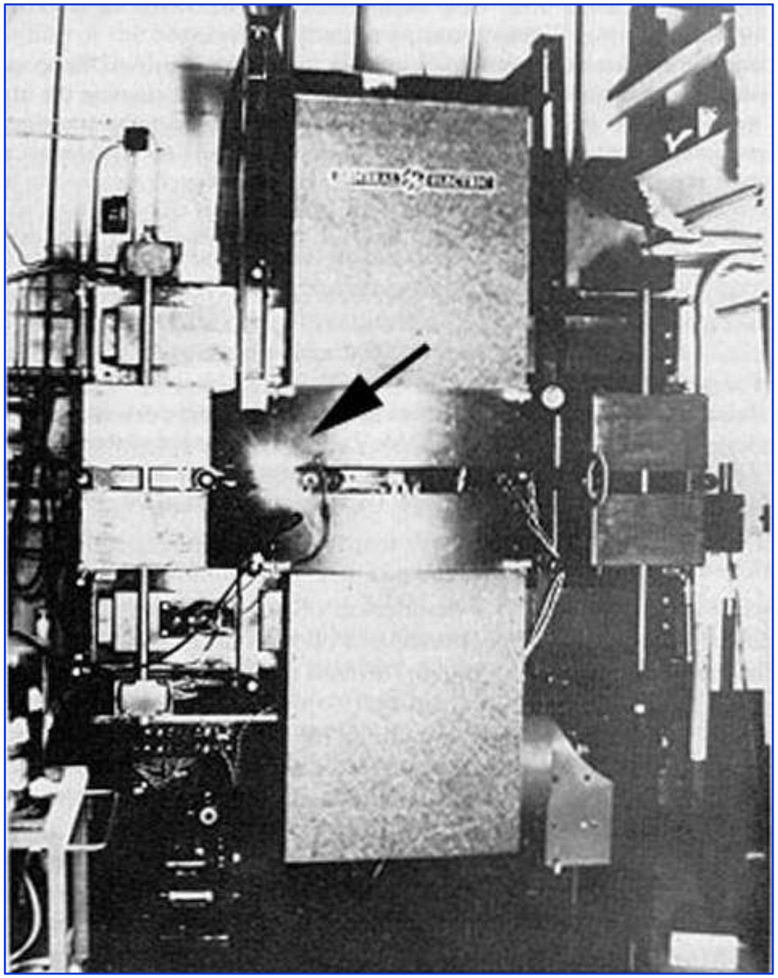


ESRF Insertion Device (ID) - Undulator

BM and ID have different characteristics concerning, spectral distribution, flux, brightness and polarization.

Short History

Synchrotron radiation: history



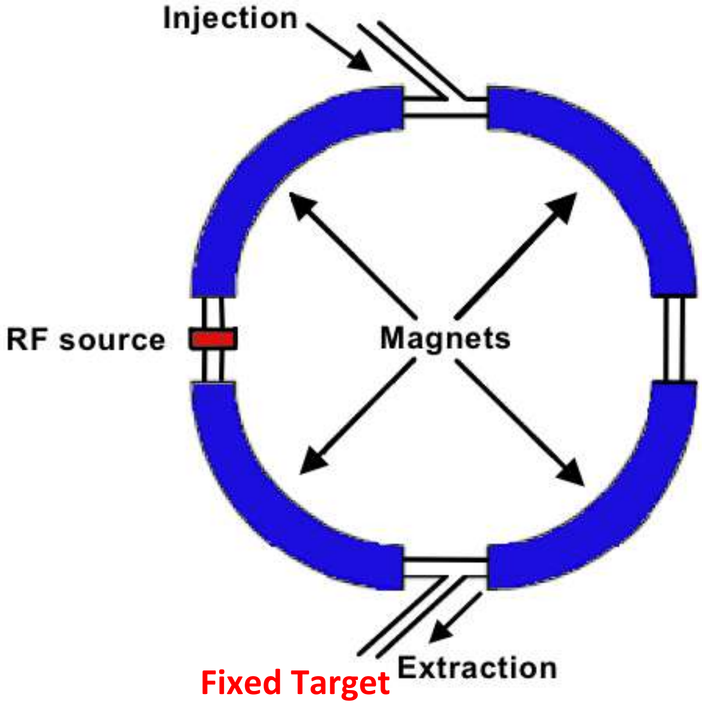
1947 *General Electric Res. Lab.* - 70 MeV Electron Synchrotron – N.Y. USA

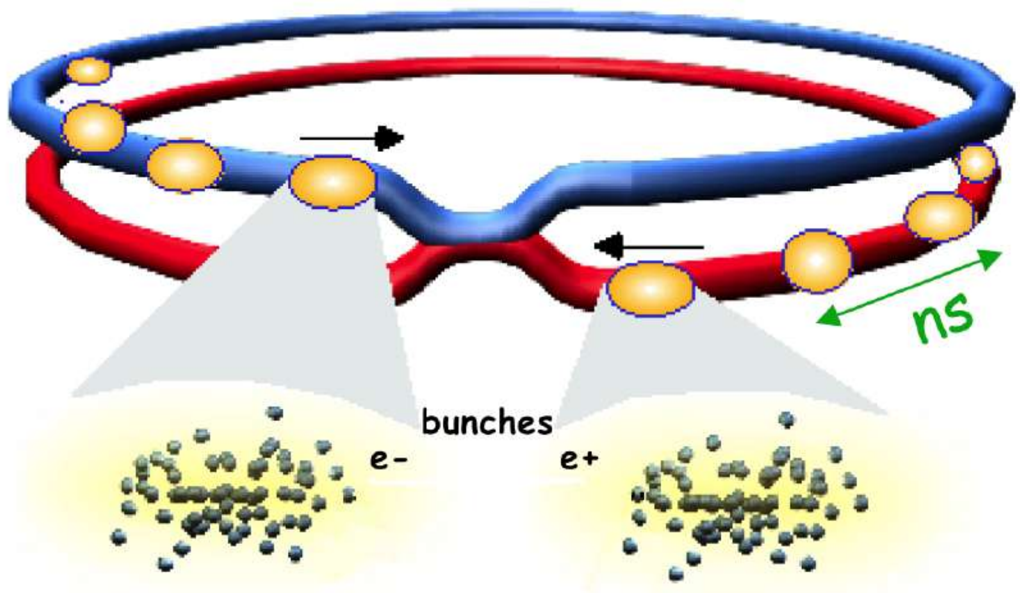
Starting point: Proof of concepts, tests of theories!

- In the 50s and 60s machines built for High Energy Physics: synchrotrons (*1947 First 'visual observation of synchrotron radiation*).
- Synchrotron radiation was considered a ***nuisance by particle physicists***: ***unwanted but unavoidable loss of energy***!
- 1961 US National Bureau of Standards (now NIST) modified their electron synchrotron : ***access to the synchrotron radiation users***.
- Synchrotron radiation scientists became ***parasites*** of nuclear physics experiments. (*1961 Frascati – CNEN Electrosynchrotron – (0.4-1.1) GeV*)
- 1968 ***First storage ring dedicated*** to synchrotron radiation research: ***Tantalus*** (University of Wisconsin) only ***bending magnets.***

F.R. Elder, A.M. Gurewitsch, R.V. Langmuir, and H.C. Pollock, Radiation from Electrons in a Synchrotron, Phys. Rev. 71,829 (1947)
G. C. Baldwin and D.W. Kerst, Origin of Synchrotron Radiation, Physics Today, **28**, 9 (*1975*)

Synchrotrons and Storage Rings





Synchrotron

Particle beam on fixed target

$E_{CM} = (mE)^{1/2}$

Storage rings

Colliding particle beams

$E_{CM} = 2E$

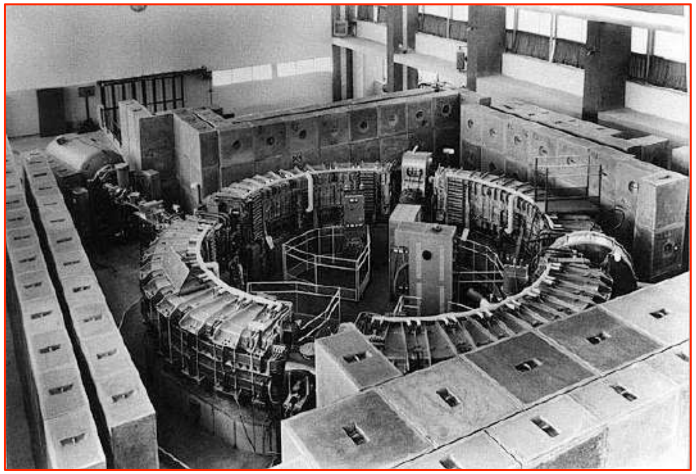
Colliding beams more efficient

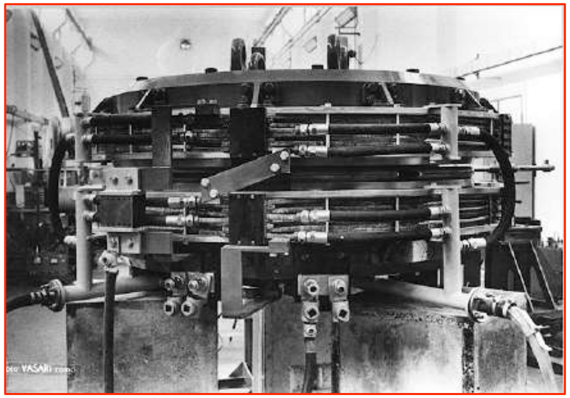
E= particle energy >> m_0c^2 *E_{CM}= center-of-mass energy*

Synchrotron radiation: short history

Frascati: ElettroSynchrotron, ADA and ADONE

Frascati - CNEN (Comitato Nazionale Energia Nucleare) Laboratory ElettroSincrotrone – (0.4-1.1) GeV, C= 28 m (1959-1975)



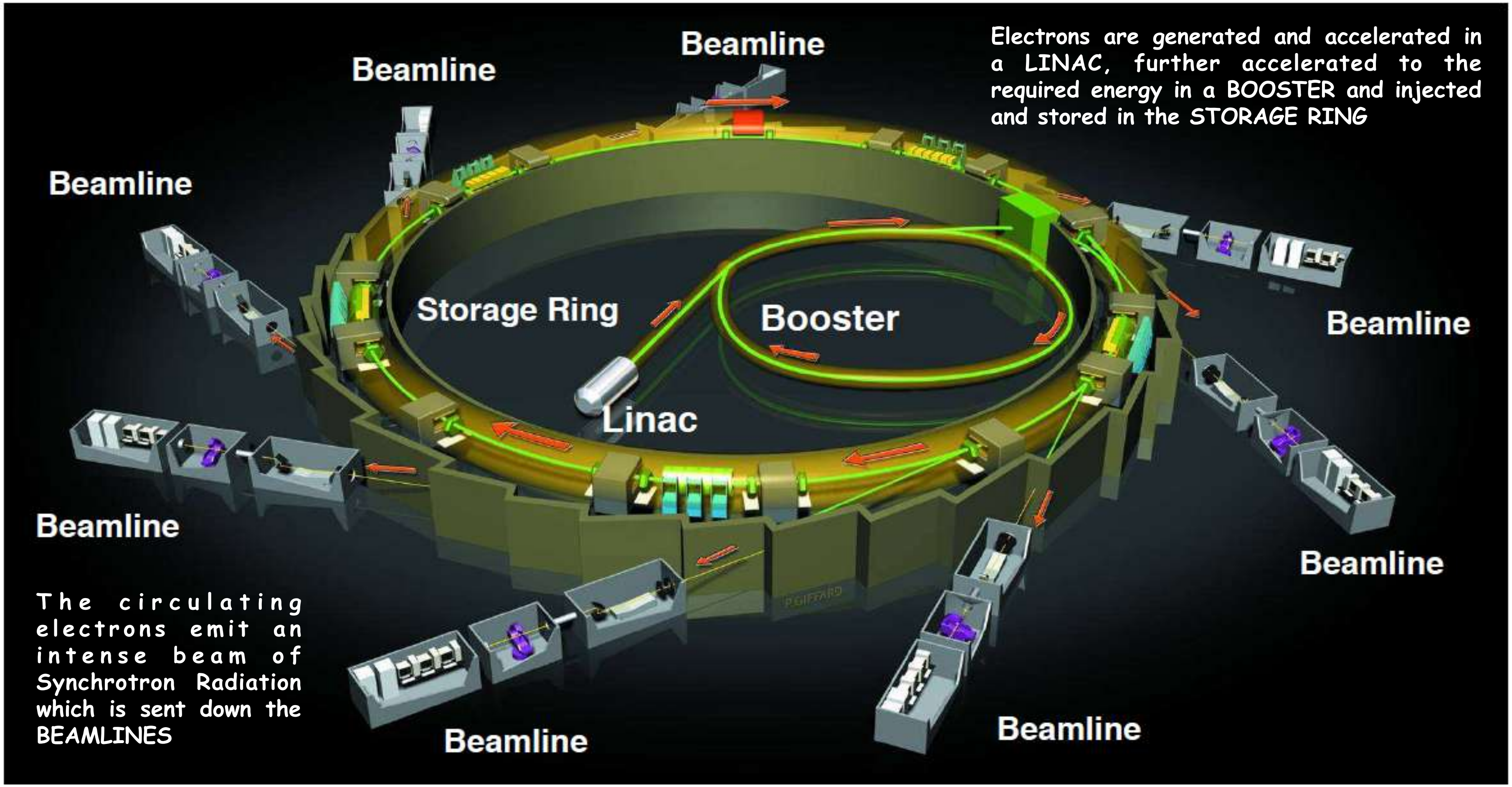


LNF ADA (Anello Di Accumulazione) – first electron-positron storage ring (proposed by B. Touschek) 0.25 GeV, C= 5 m (1961-1964)

LNF ADONE (big ADA) electron-positron storage ring 1.5 GeV per beam, C = 105 m (1969-1993)

1976-1993 LNF ADONE 1.5 GeV parasitic/dedicated use for SR experiments after its use for HE experiments.

Schematic view of a Synchrotron Radiation facility



As a function of the energy range to be used each beamline must be optimized for a particular field of research.

Beamline schematic composition:

- *Front end*
- *Optical hutch*
- *Experimental hutch*
- *Control and computing*

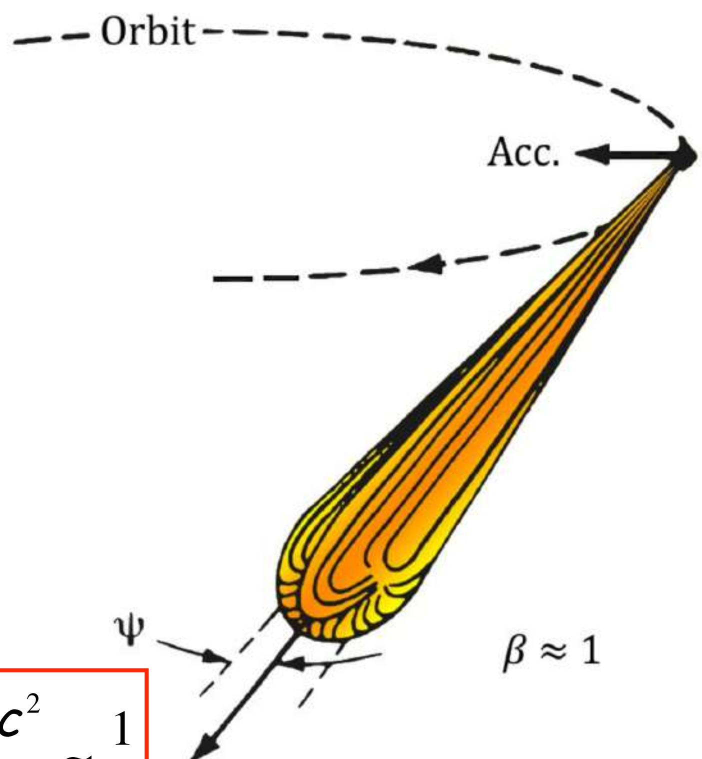
The ***front end*** isolates the beamline vacuum from the storage ring vacuum; **defines the angular acceptance of the synchrotron radiation** via an aperture; blocks(beam shutter) when required, the x-ray and Bremsstrahlung radiation during access to the other hutches.

Synchrotron radiation properties

Synchrotron radiation: physics

Relativistic focusing of Synchrotron Radiation

For a ***relativistic effect***, when the speed of the emitting electrons increases to relativistic values ($v \approx c$) the radiation pattern is compressed into a ***narrow cone in the direction of motion, resulting into an emission tangential to the particle orbit***.



$$\psi \approx \frac{m_0 c^2}{E} \approx \frac{1}{\gamma}$$

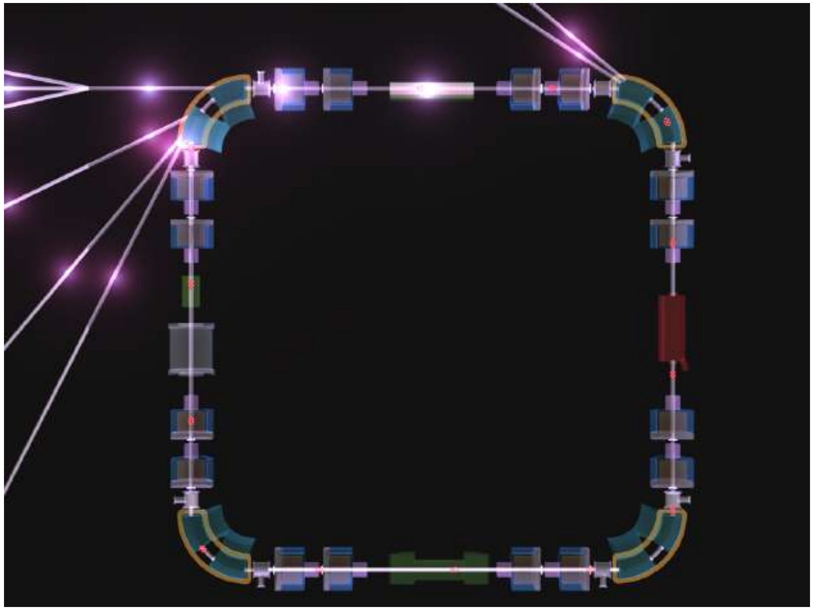
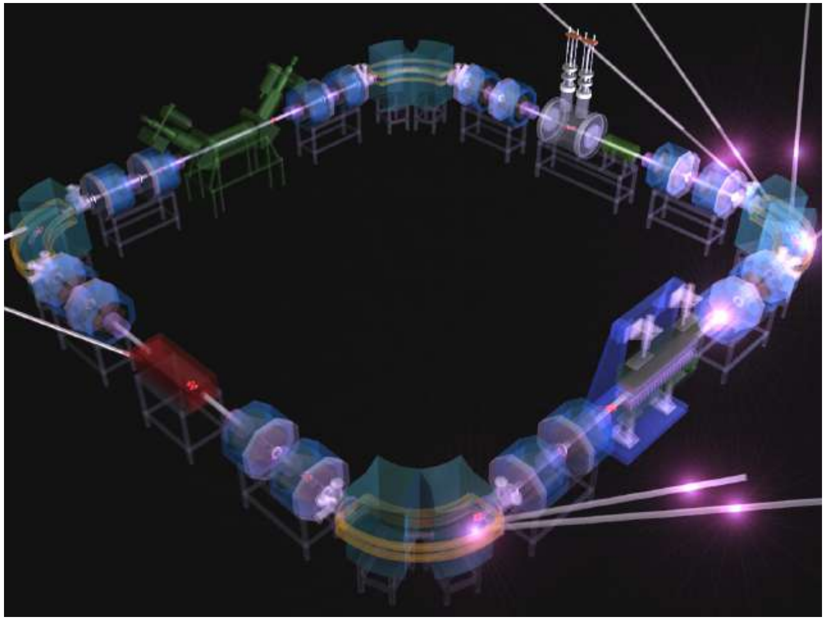
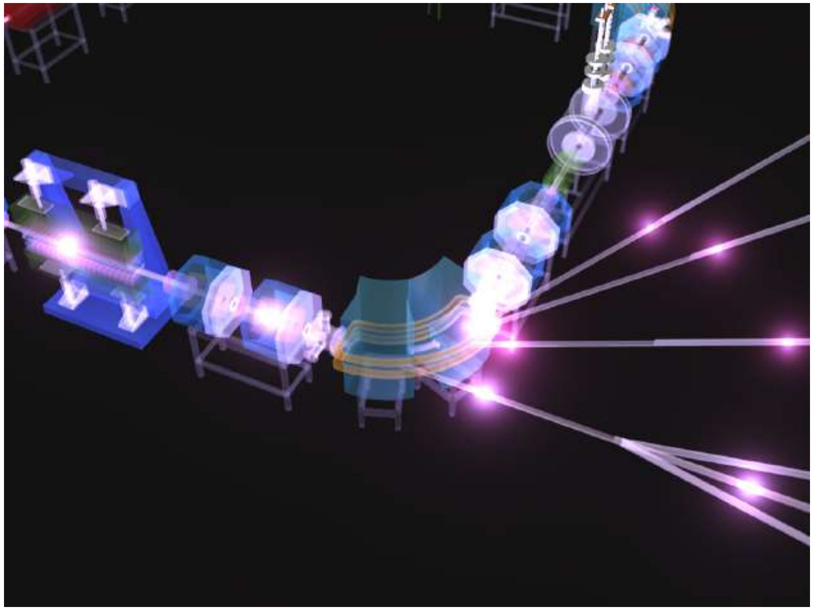
$v \approx c$ or $\beta = v/c \approx 1$

Radiated power:

$$P_{rad} = \frac{2}{3}\frac{Q^2 c}{R^2}\left[\frac{E}{m_0 c^2}\right]^4$$

Q = particle charge, ***E*** = particle energy, m_0 = rest mass, ***R*** = radius of curvature

1949 Schwinger: classical theory of radiation from accelerated relativistic electrons

ASTRID (Aarhus - Denmark) http://www.isa.au.dk/animations/pictures/pic-index.asp

http://www.isa.au.dk/animations/Finalmovie/astrid_total_v2.mov

Synchrotron Radiation Properties

What makes synchrotron radiation interesting, powerful and unique?

- ***Continuum source from IR to X-rays*** ***(tunability)*** which covers from **microwaves to hard X-rays**: the user can select the wavelength required for experiment- **continuous** *(Bending Magnet/Wiggler)* - **quasi-monochromatic** *(Undulator)*

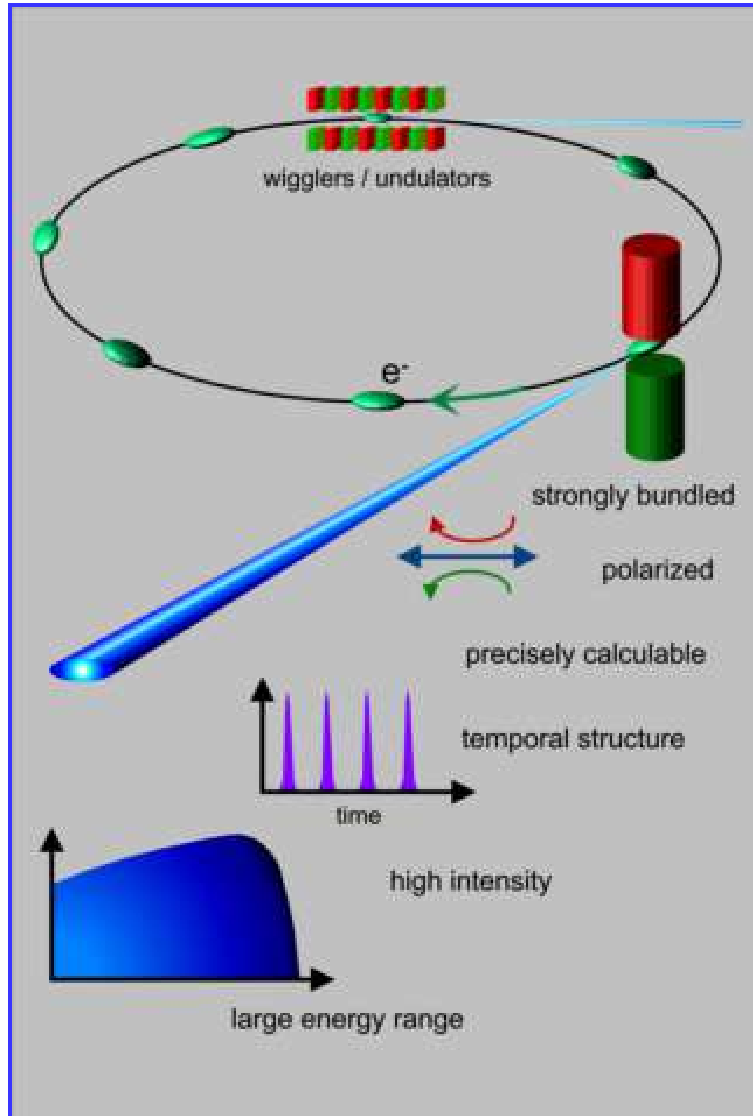
- ***Source in a clean UHV environment***

- ***Very high flux and brightness (with undulators)*** highly **collimated photon beams** generated by a ***small divergence*** and **small size sources** .

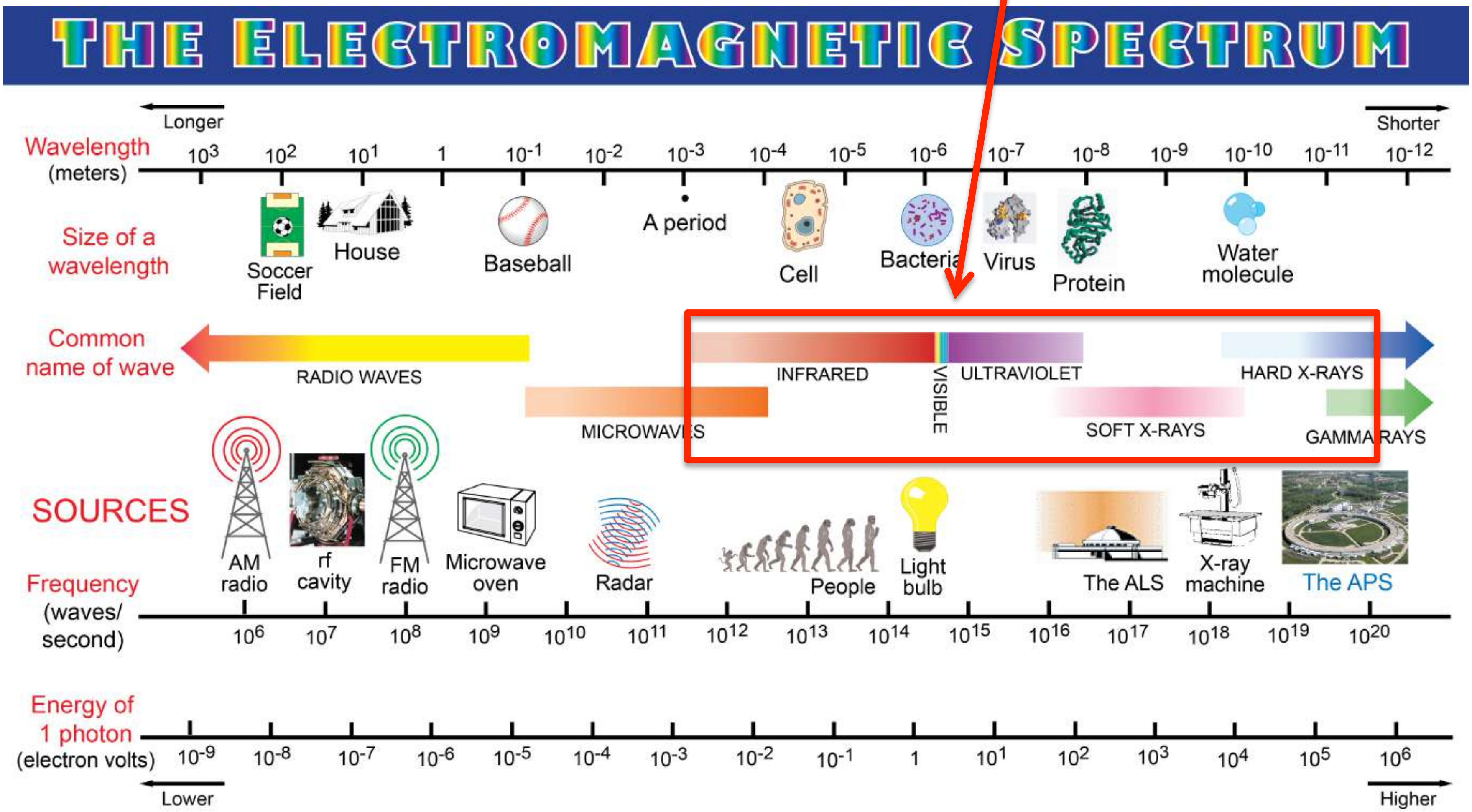
- ***Highly Polarized***

- ***Pulsed time structure*** **-** pulsed length down to tens of picoseconds allows the resolution of processes on the same time scale

- ***High stability*** **(submicron source stability)**



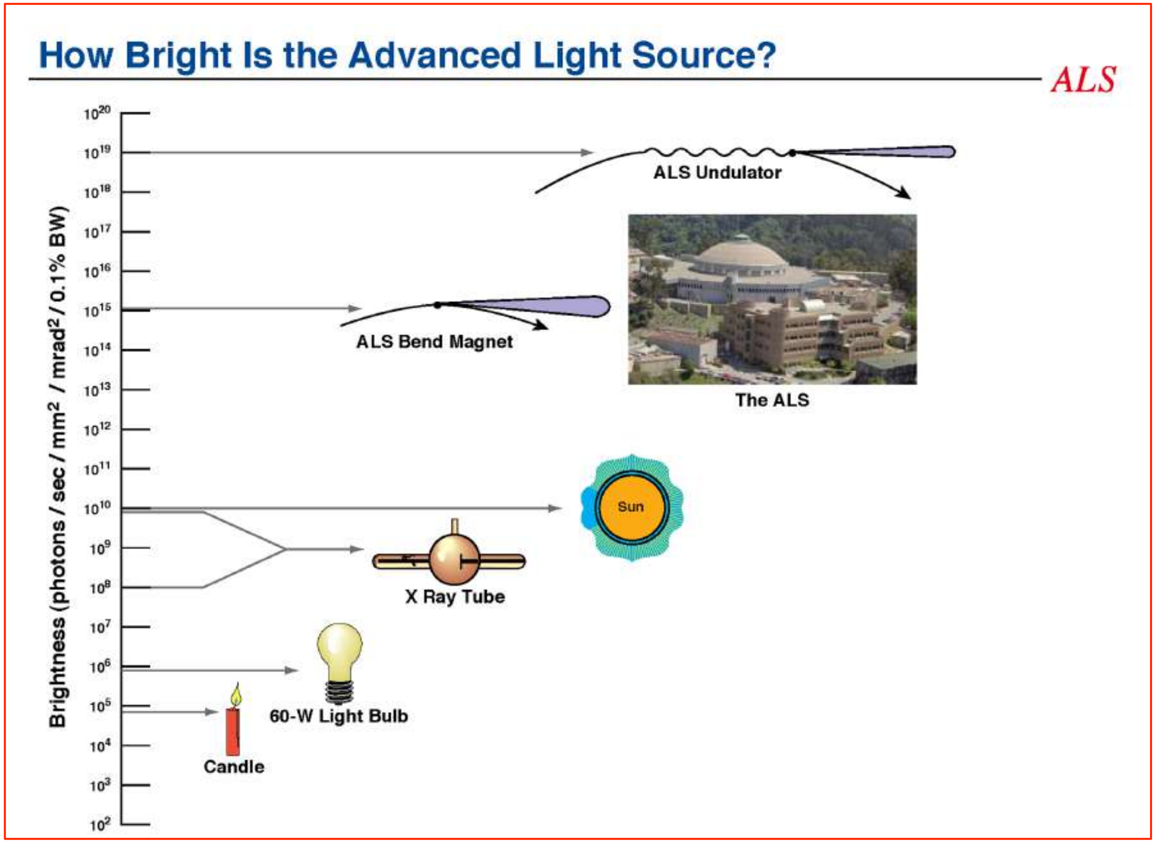
Spectral range covered by Synchrotron Radiation!



Brightness

Brightness

Synchrotron radiation sources have very high brightness.

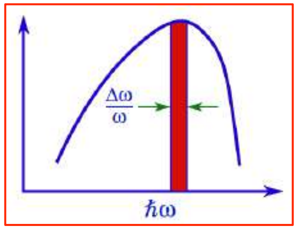


Brightness of third generation low emittance storage rings.

- ***Electrons in vacuum*** *can emit more power than electrons in a solid because the power does not damage their environment ⇒* ***high flux.***
- *The* ***source size*** *is not that of a single electron but the transverse cross section of the electron beam. The sophisticated trajectory control system makes it* ***very small.***
- *Relativity induces* ***drastically reduced angular divergence*** *of the emission.*

Spectral brightness is that portion of the brightness lying within a ***relative spectral bandwidth*** $\Delta\omega/\omega$:

$$\text{Spectral Brightness} = \frac{\text{photons}}{\text{second} \cdot \text{mrad}^2 \cdot \text{mm}^2 \cdot 0.1\%\text{BW}}$$



3rd Generation Light Sources

ESRF - France

DIAMOND - UK

ALBA - Spain

Brightness is the main figure of merit of synchrotron radiation sources and its huge increase, was obtained designing low emittance machines, minimizing the source size and the beam divergence.

Ultimate SR facilities

Lund - Sweden

Sirius - Brazil

Shanghai -China

Synchrotron radiation @ INFN-Frascati National Laboratory

DAΦNE Light

Synchrotron Radiation Facility

DAΦNE-Light

INFN-LNF Synchrotron Radiation Facility

Beamlines @ DAΦNE

1) SINBAD - IR beamline (1.24 meV - 1.24 eV)

2) DXR1- Soft x-ray beamline (900-3000 eV)

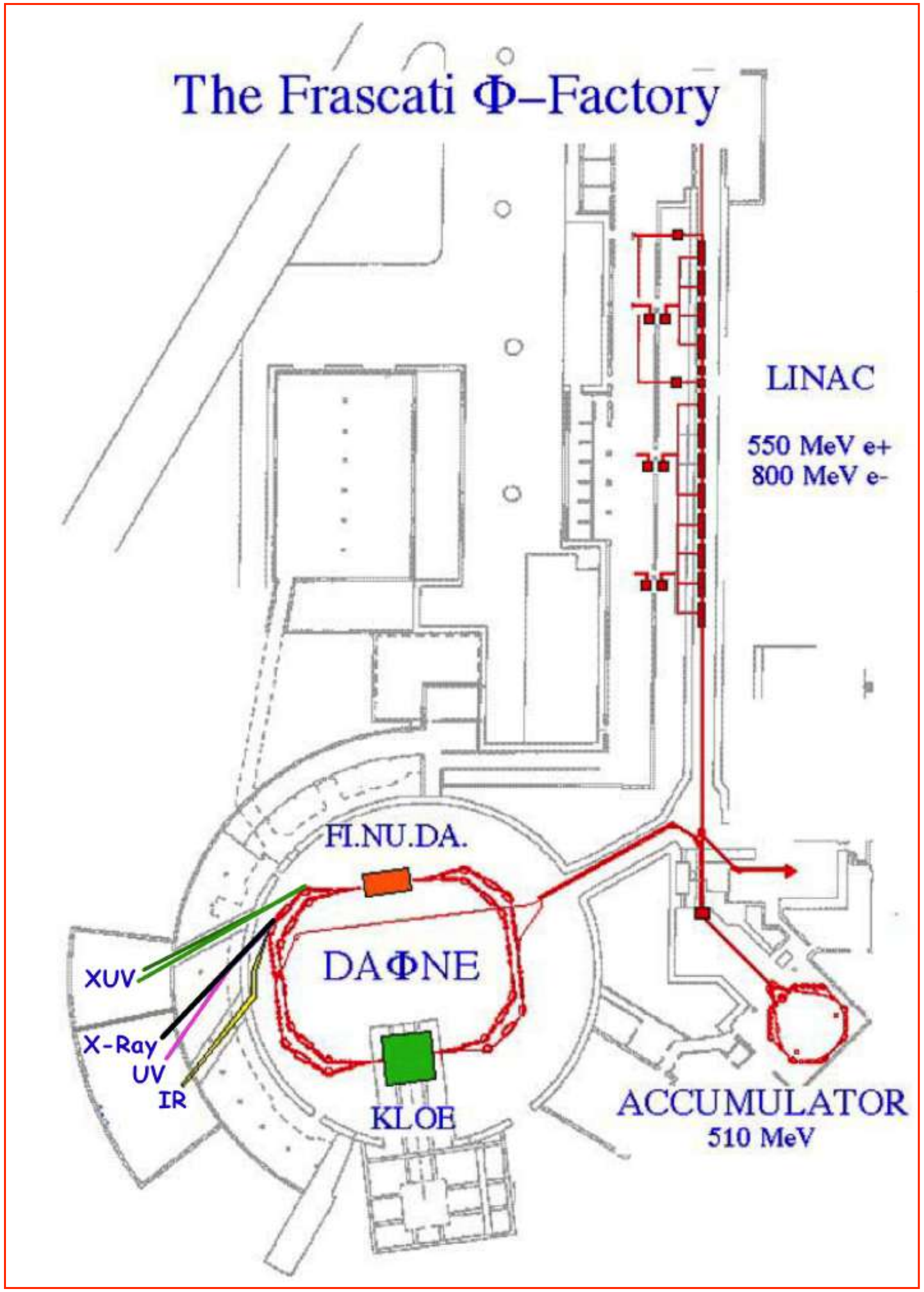
Open to Italian and EU users

3) DXR2 – UV-VIS beamline (2-10eV) new setup.

XUV beamlines

4) Low Energy Beamline (35-200 eV) ready for commissioning;

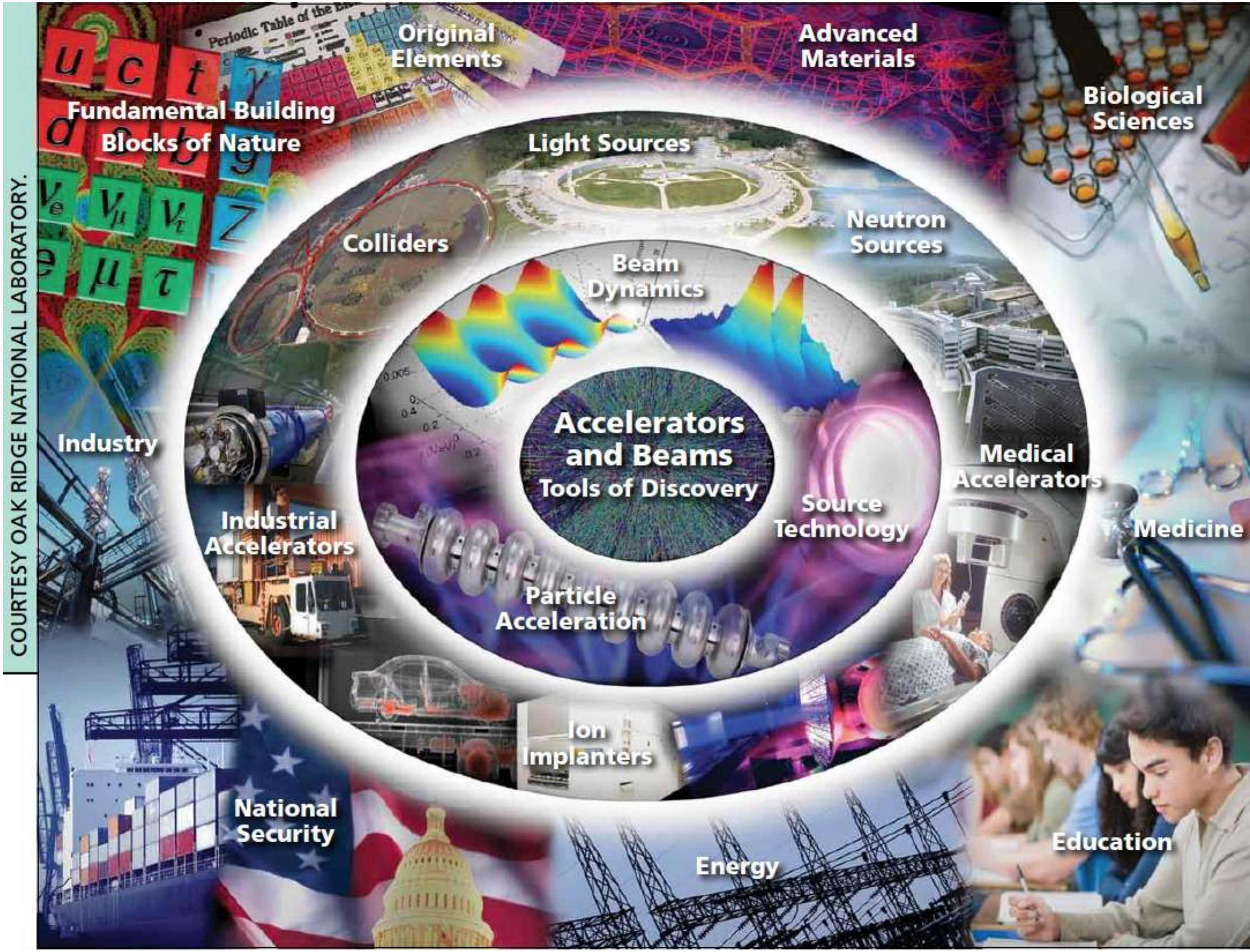
5) High Energy Beamline (60-1000eV) ready for commissioning.



Available techniques

- FTIR spectroscopy, IR microscopy and IR imaging
- UV-Vis absorption spectroscopy
- Photochemistry: UV irradiation and FTIR micro-spectroscopy and imaging.
- Soft x-ray spectroscopy: XANES (X-ray Absorption Near Edge Structure) light elements from Na to S
- SEY (secondary electron yield) and XPS (X-ray photoelectron spectroscopy) – by electron and photon bombardment

From accelerators to applications

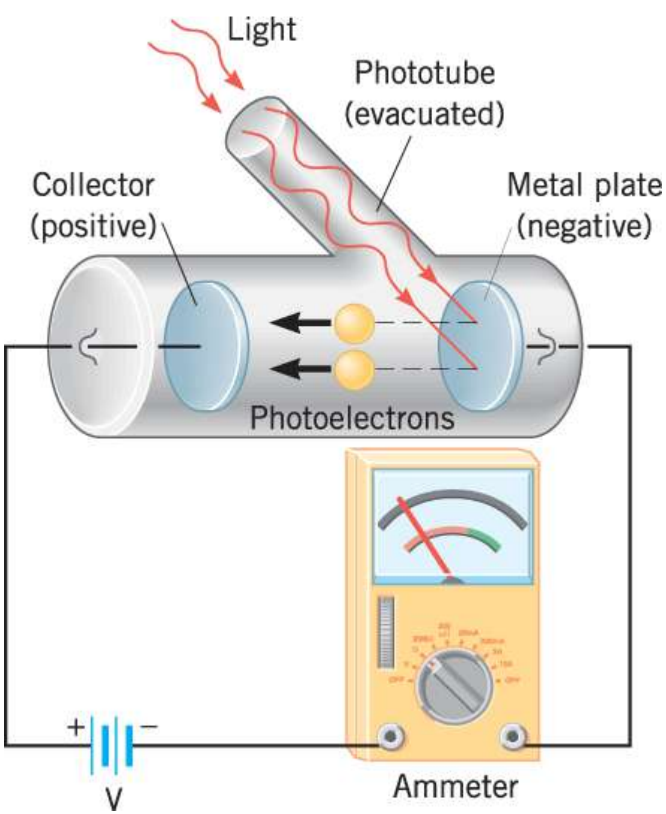


E. Malamud Ed., ***Accelerators and Beams tools of discovery and innovation*** (http://www.aps.org/units/dpb/news/edition4th.cfm) ***2013***

Interactions of x-rays with matter

Photoelectric effect

Electromagnetic radiation can be used to push electrons, freeing them from the surface of a solid. This process is called the ***photoelectric effect*** (or ***photoelectric emission*** or ***photoemission***), a material that can exhibit this phenomena is said to be ***photoemissive***, and the ejected electrons are called ***photoelectrons***; but there is nothing that would distinguish them from other electrons. All electrons are identical to one another in mass, charge, spin, and magnetic moment.

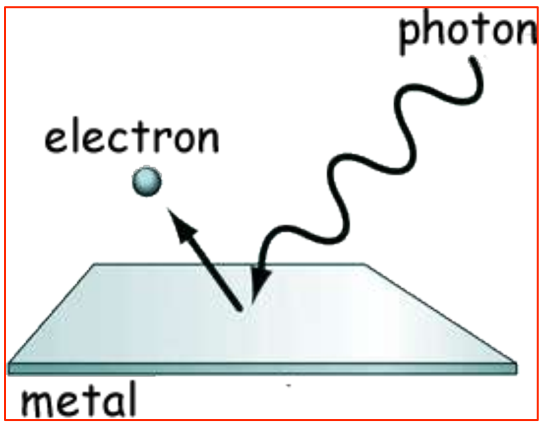


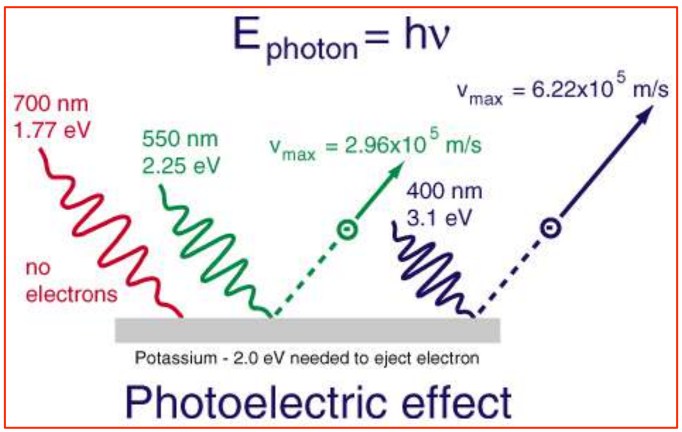
The photoelectric effect does not occur when the frequency of the incident light is less than the ***threshold frequency***. ***Different materials have different threshold frequencies***.

Photoelectric effect

Classical physics cannot explain why…
- **no photoelectrons are emitted when the incident light has a frequency below the threshold,**
- **the maximum kinetic energy of the photoelectrons increases with the frequency of the incident light,**
- **the maximum kinetic energy of the photoelectrons is independent of the intensity of the incident light**, and
- **there is essentially no delay between absorption of the radiant energy and the emission of photoelectrons**.

Modern physics states that…
- **electromagnetic radiation is composed of discrete entities called photons**
- **the energy of a photon is proportional to its frequency**
- **the work function of a material is the energy needed per photon to extract an electron from its surface**

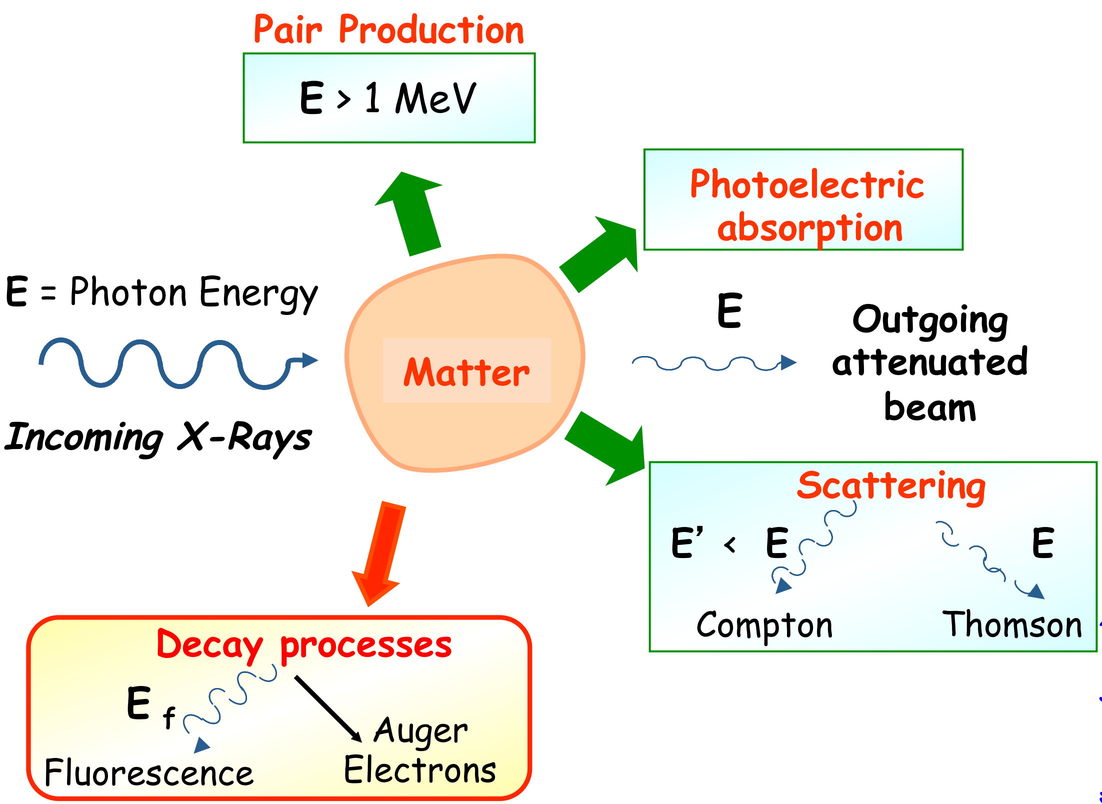


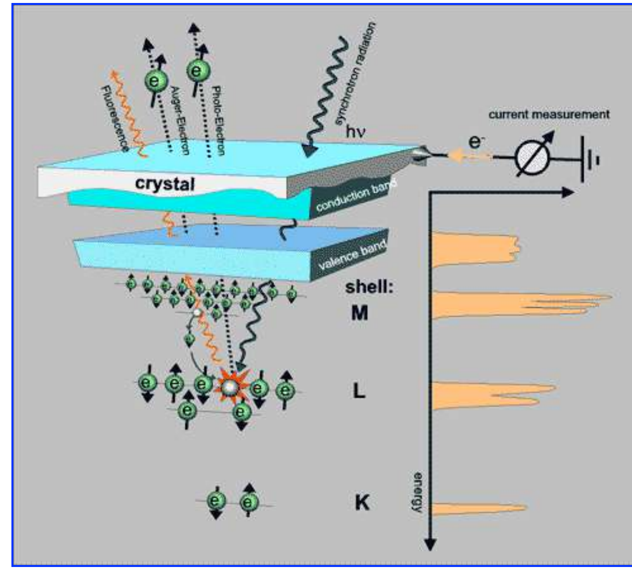


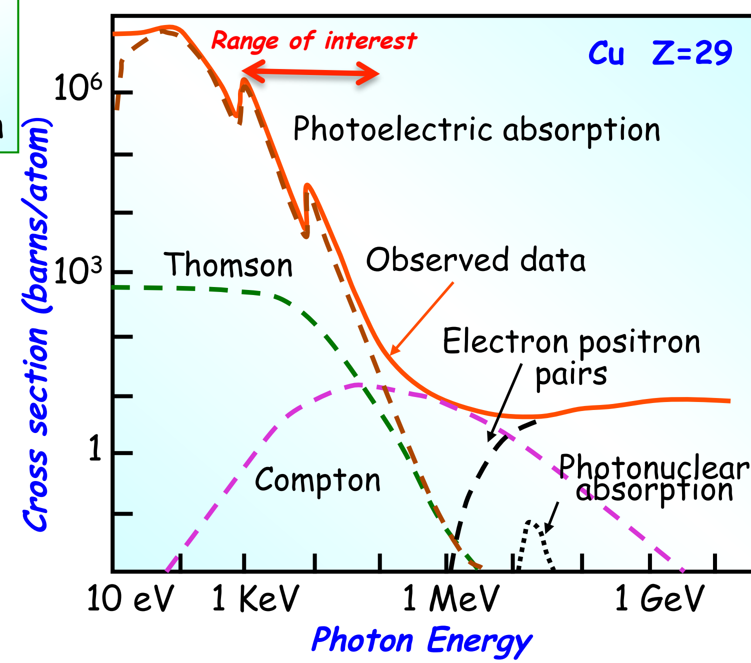
In 1905, ***Albert Einstein realized that light was behaving as if it was composed of tiny particles*** (initially called quanta and later called photons) and that **the energy of each particle was proportional to the frequency of the electromagnetic radiation** (**Nobel Prize in Physics in 1921**).

Interaction of X-rays with matter

Attenuation mechanisms for X-rays



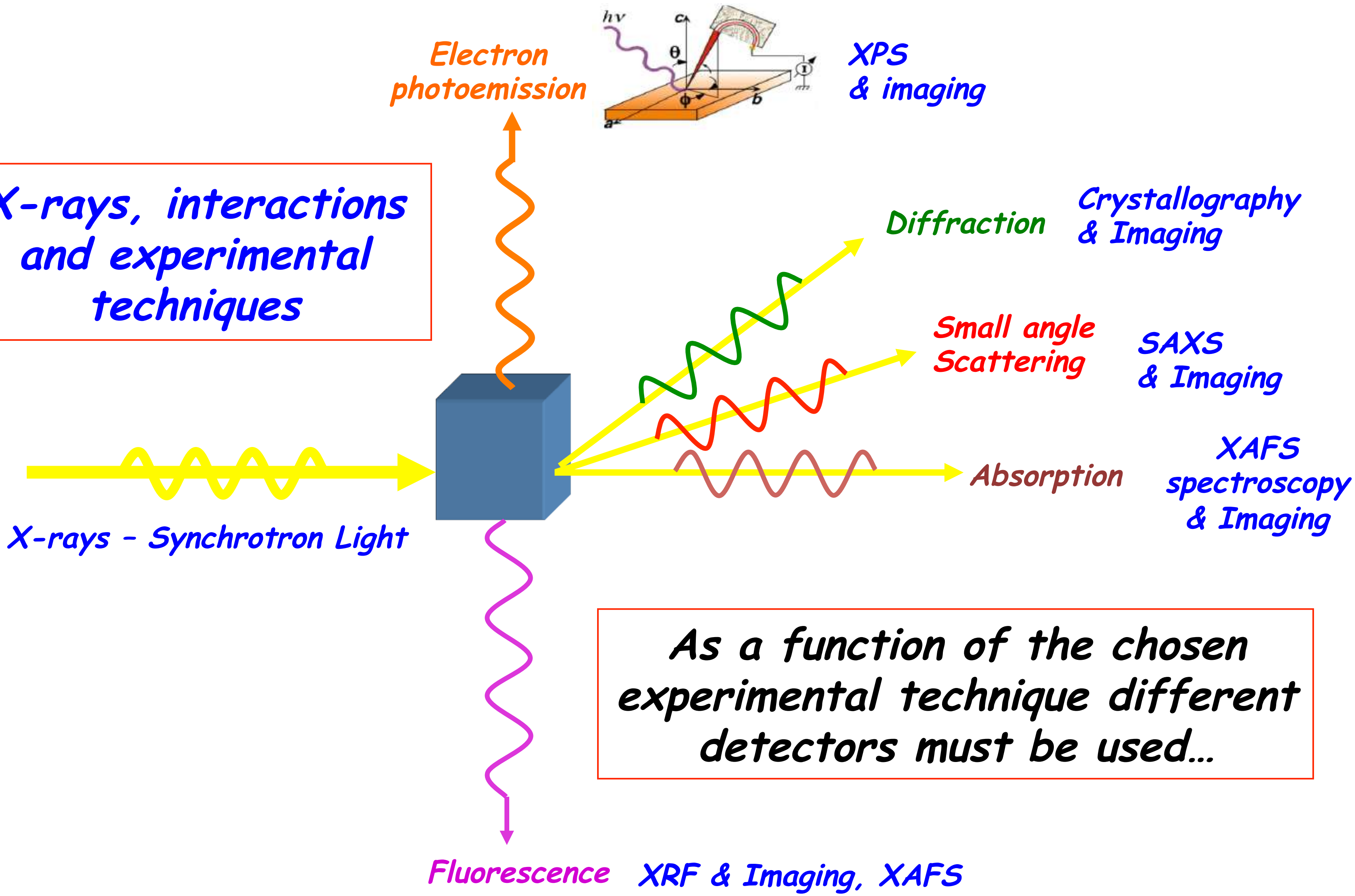




There are different types of interaction of X-rays with matter but taking into account the energy range of interest the one that will be taken into account is *x-ray absorption*.

X-rays interactions with matter and experimental techniques

X-rays, interactions and experimental techniques

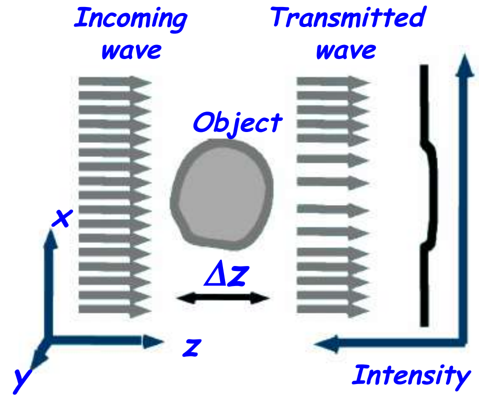


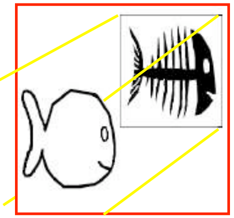
As a function of the chosen experimental technique different detectors must be used…

Some X-ray techniques

Imaging

Conventional radiology relies on X ray absorption

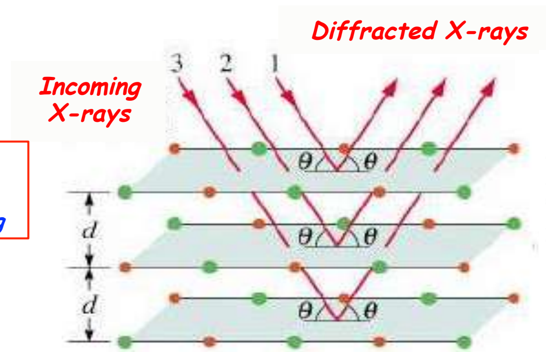


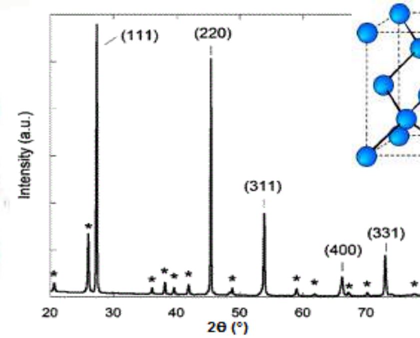


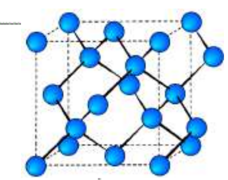
Scattering

Elastic scattering : Thomson (elastic) if $E<E_{binding}$

$$n\lambda=2d\sin\theta \quad \text{Bragg's Law}$$





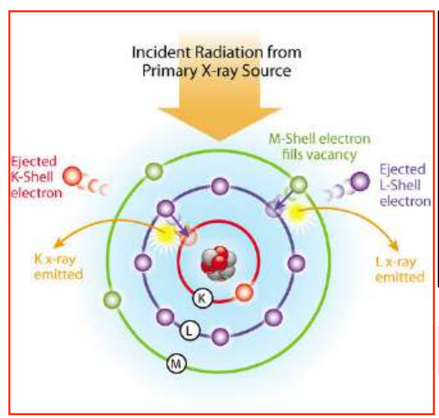


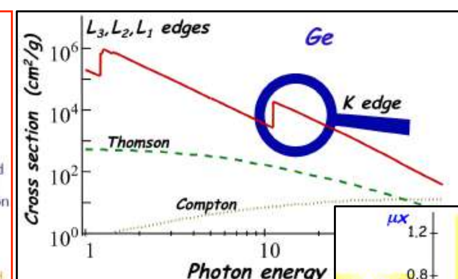
Ge crystal structure

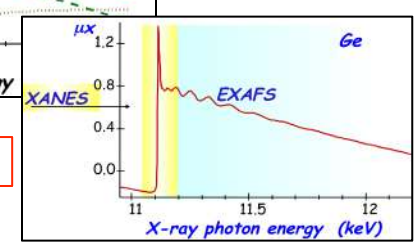
Spectroscopy

X ray Absorption Fine Structure (XAFS)

Transmission and fluorescence mode







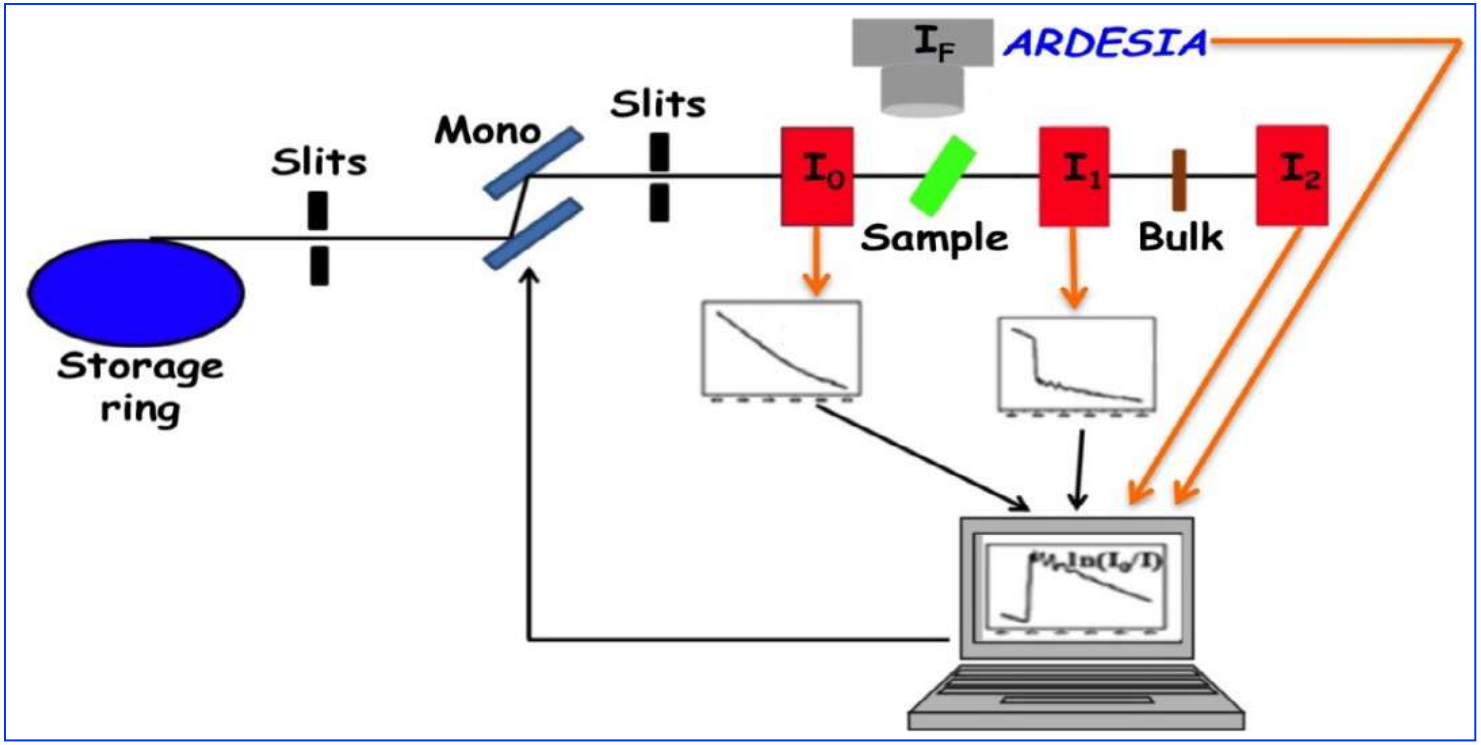
XAFS=XANES+EXAFS

X-ray Absorption Spectroscopy

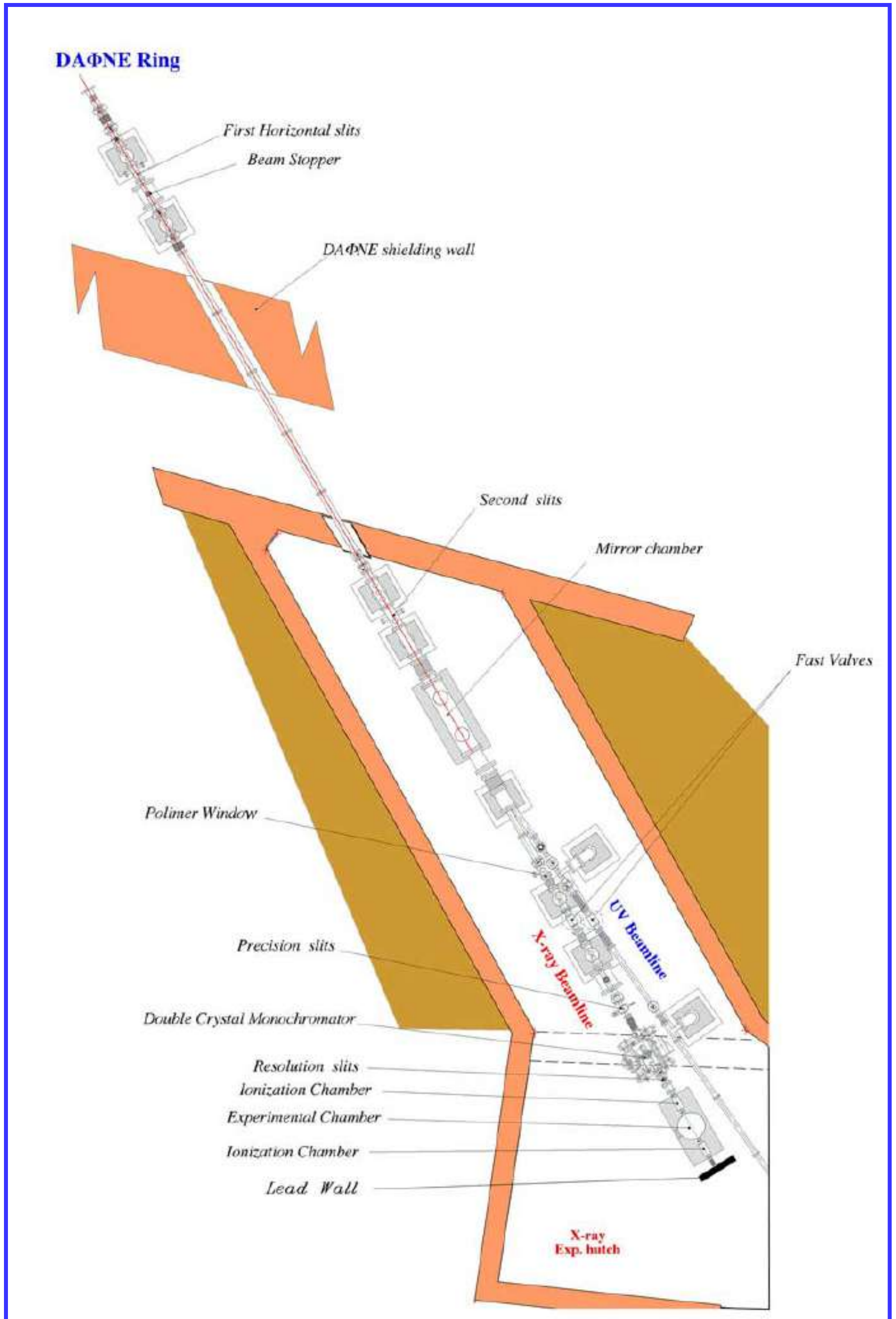
XAS local sensitive and chemical selective probe
that can provide structural, electronic and magnetic information.

XAFS beamline

DAFNE-L DXR1 beam line absorption spectroscopy



I_0, I_1, I_2 Gas ionization chambers - I_F SDD solid state detector

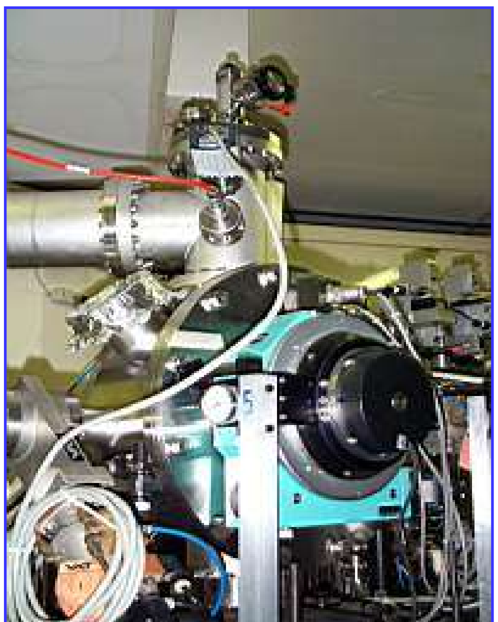


DAΦNE Soft X-ray DXR1 Beamline

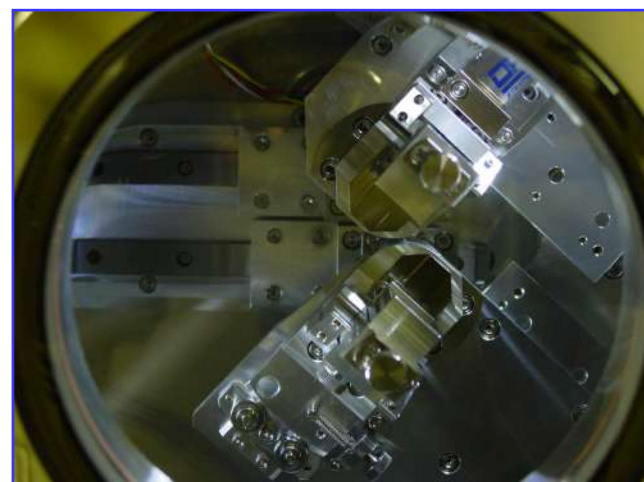
- *Wiggler soft x-ray beam line*
- *Critical energy E_c = 284 eV*
- *Working range 0.9 - 3.0 keV*
- *TOYAMA double crystal monochromator with KTP (011), Ge (111), Si (111), InSb (111) and Beryl (10-10) crystals*
- *Soft X-ray absorption spectroscopy and tests of Soft x-ray optics and detectors.*

DXR1 Beamline

As a function of the energy range to be used each beamline must be optimized for a particular field of research.
The front end isolates the beamline vacuum from the storage ring vacuum; defines the angular acceptance of the synchrotron radiation via an aperture; blocks (beam shutter) when required, the x-ray and Bremsstrahlung radiation during access to the other hutches.

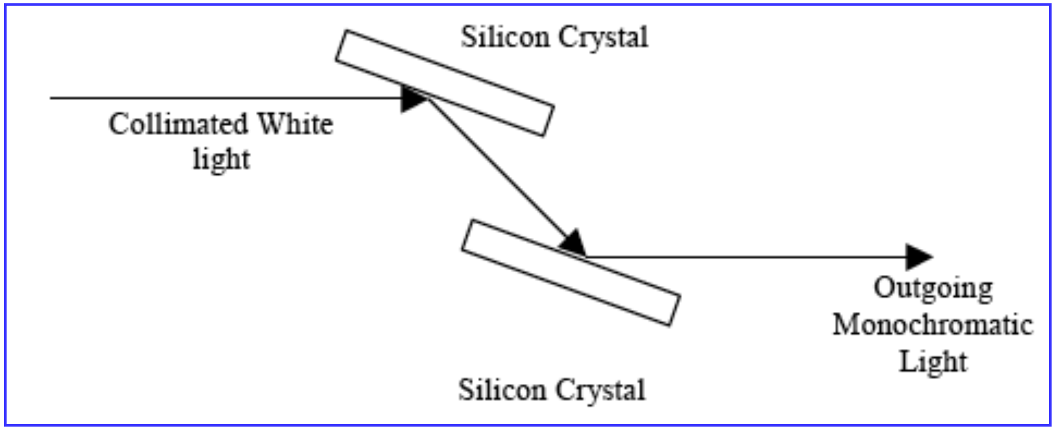


Monochromator

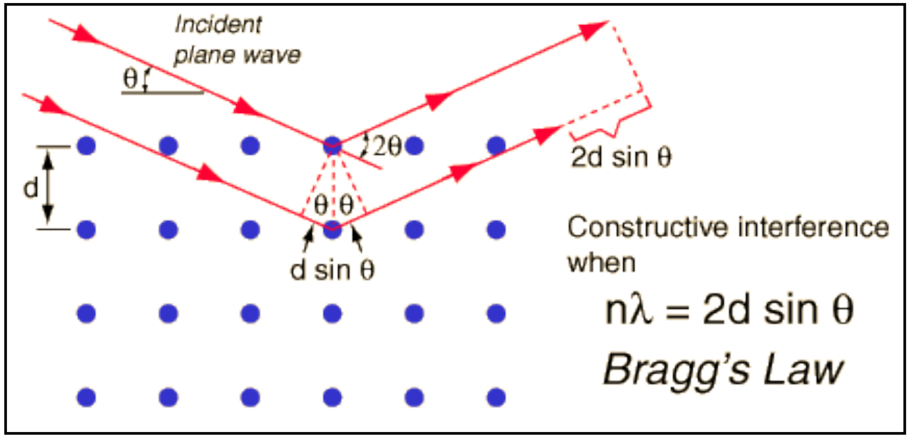


Monochromator

Prism and visible light



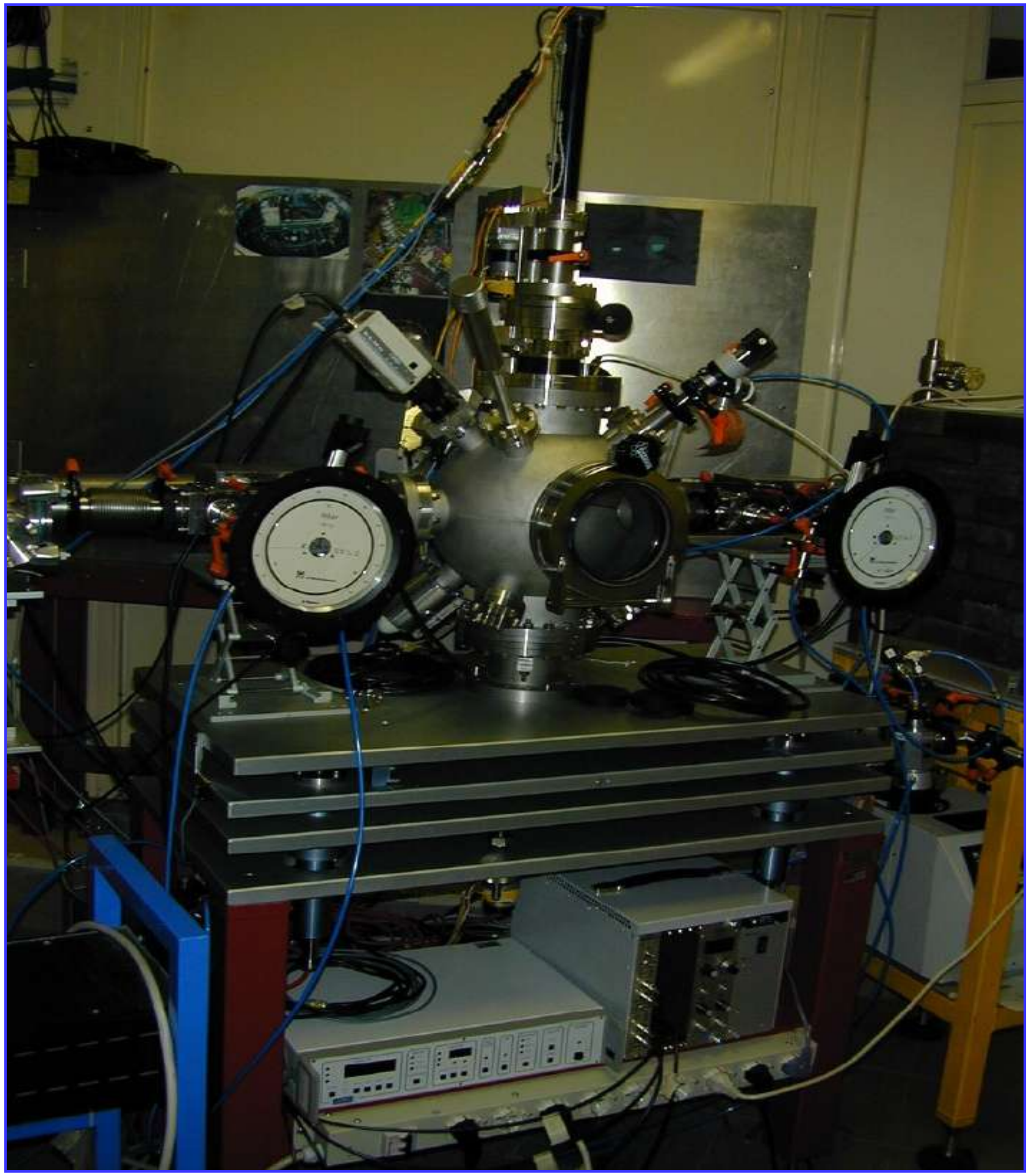
X-rays and crystals



Crystal type	2d spacing (Å)	Energy range (eV)	Absorption edges
Beryl (10-10)	15.954	1000 - 1560	Na K, Mg K, Cu L
KTP (011)	10.950	1200 - 2200	Mg K, Al K
InSb (111)	7.481	1800 - 3100	Si K, P K, S K, Cl K
Ge (111)	6.532	2100 - 3100	P K, S K, Cl K

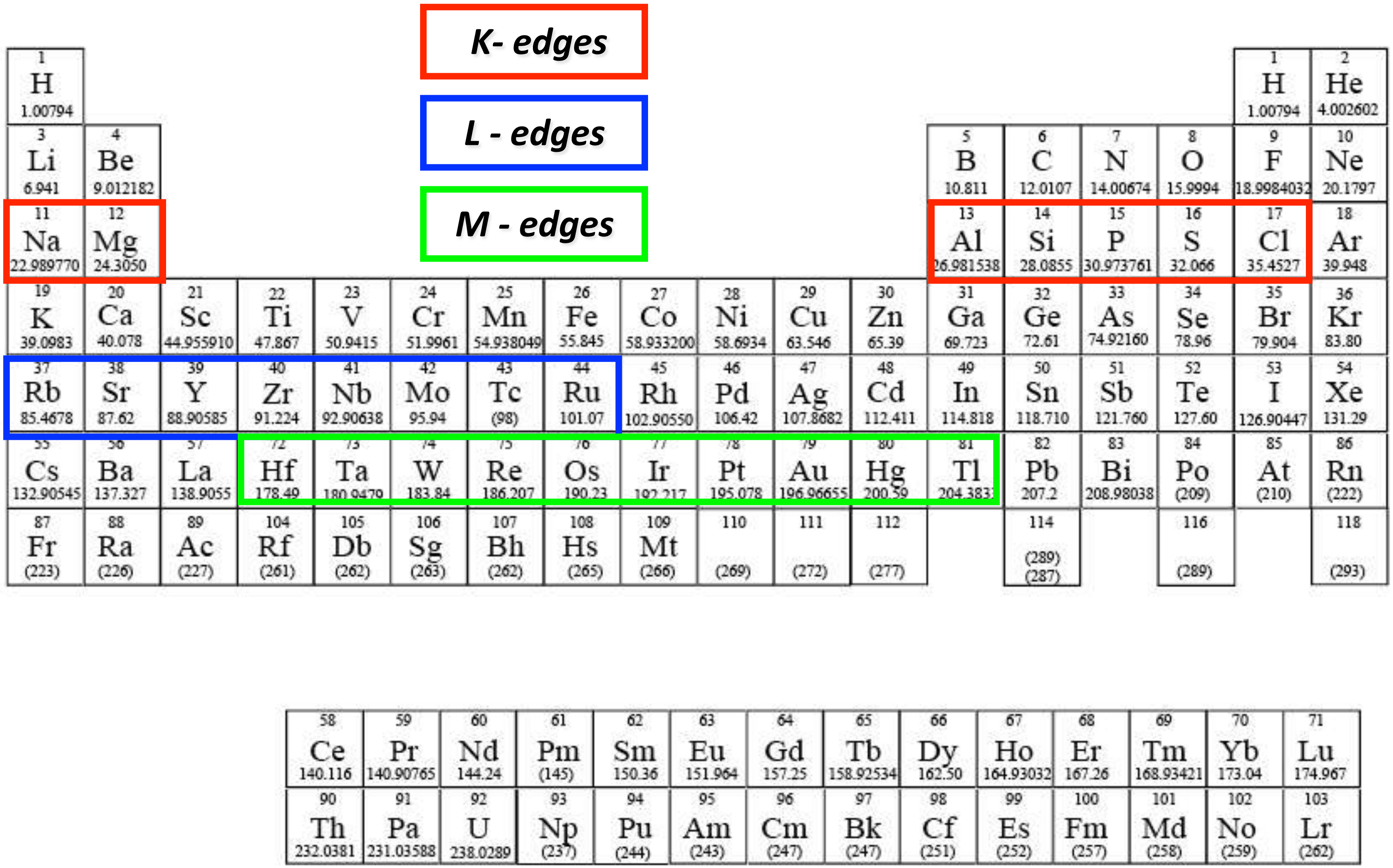
$$n\lambda = 2d\sin\theta$$ *Bragg's Law*

DXR1 Beamline

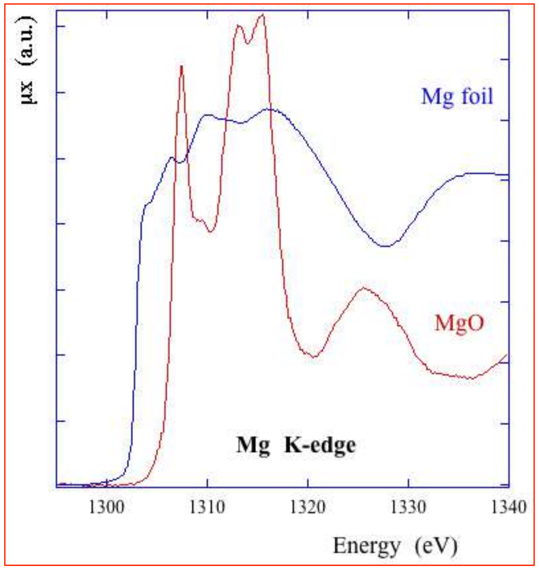


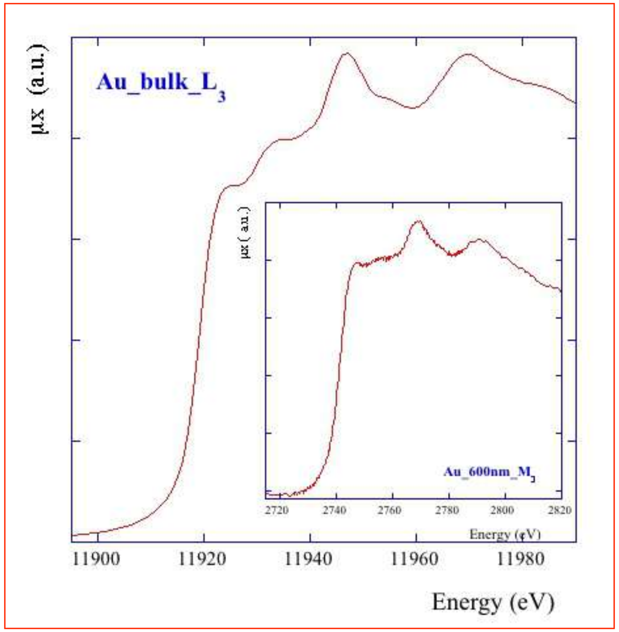
Detectors and experimental chamber

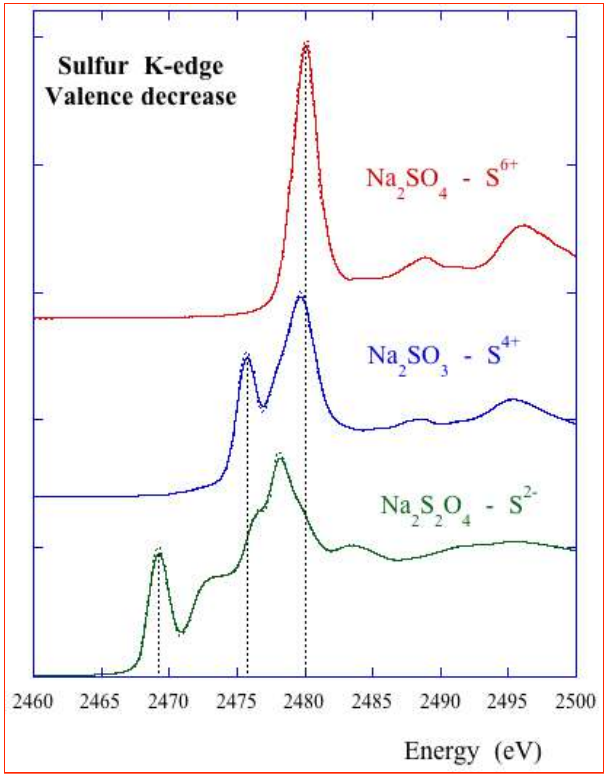
Elements that can be investigated

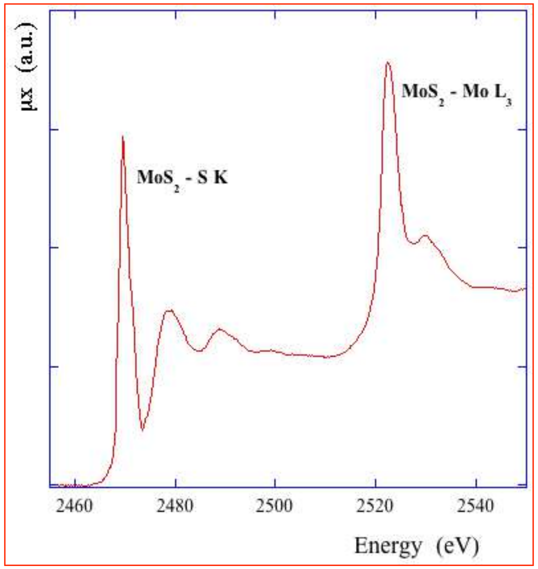


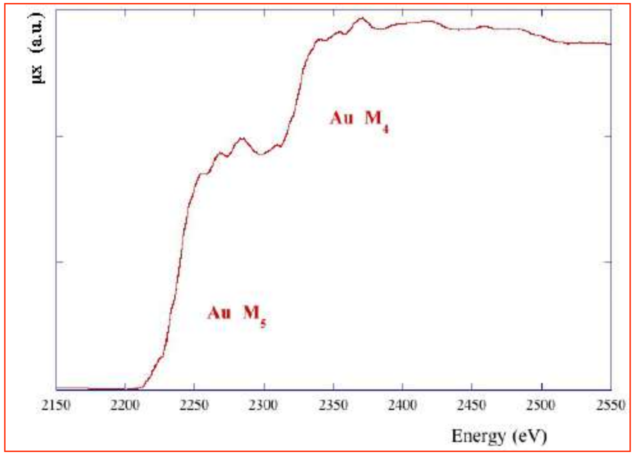
XANES examples

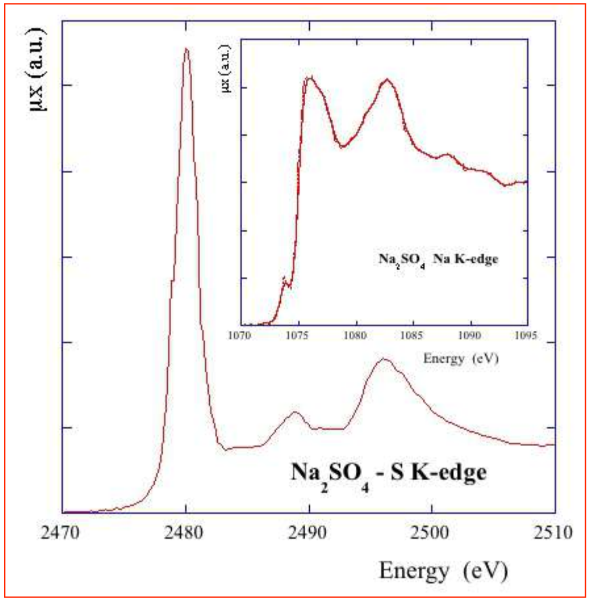




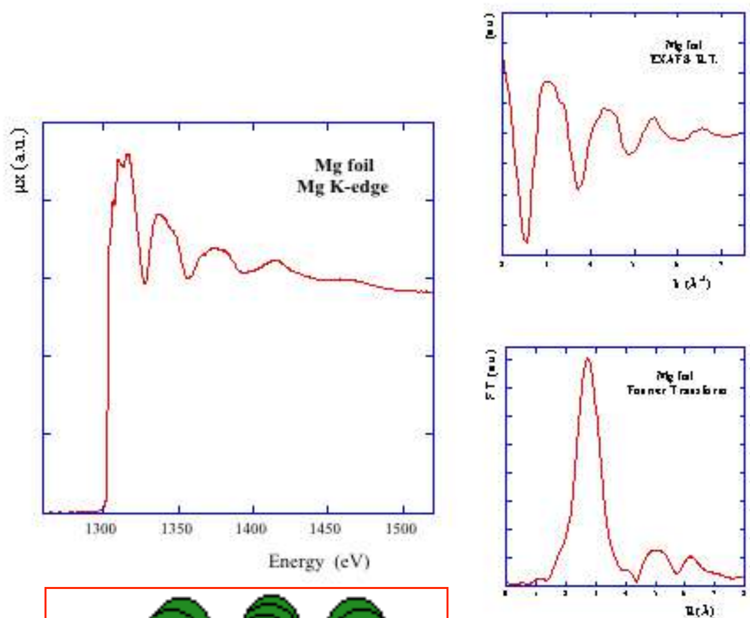


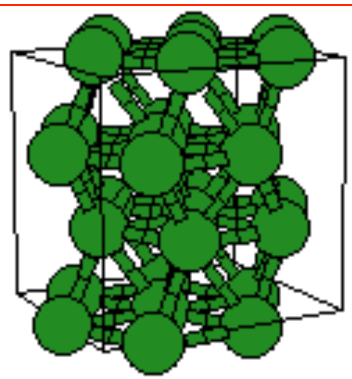




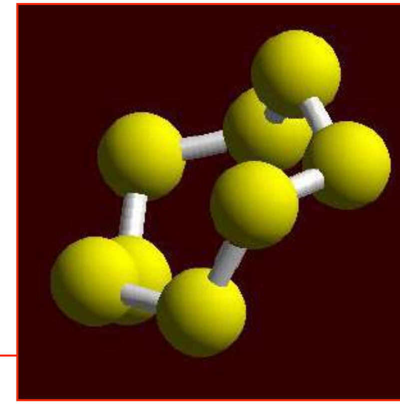


EXAFS examples

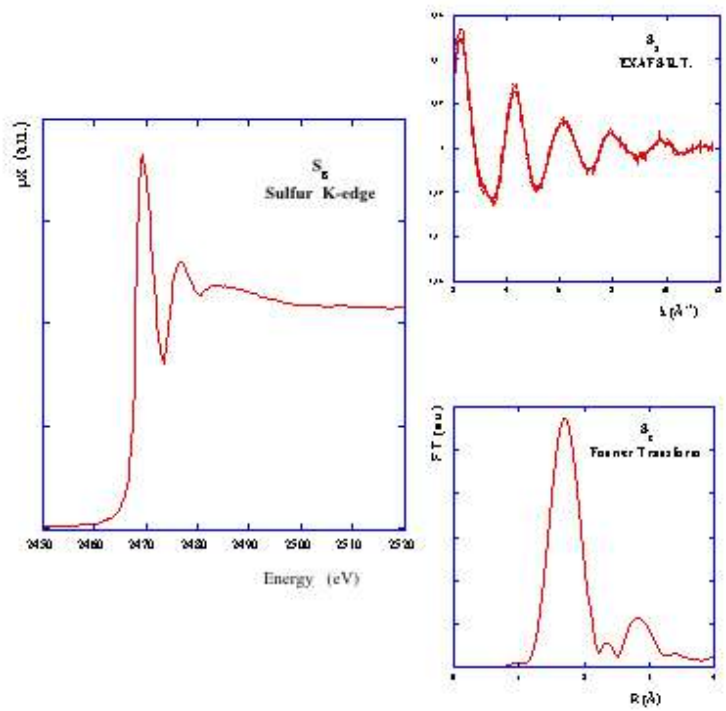




Mg hcp crystal structure

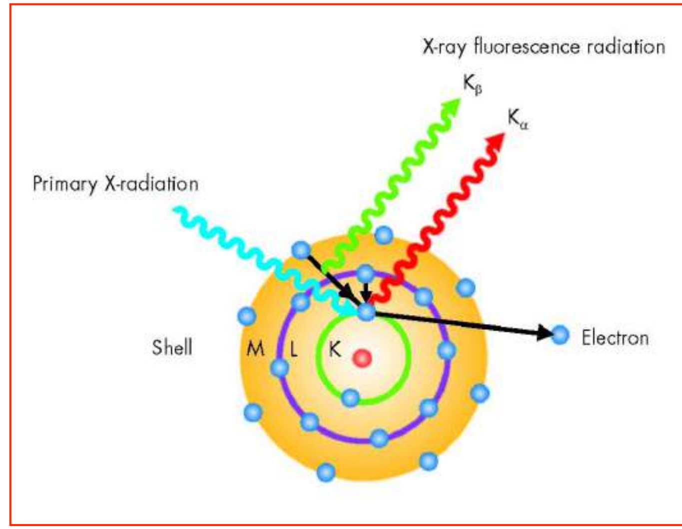


S_8

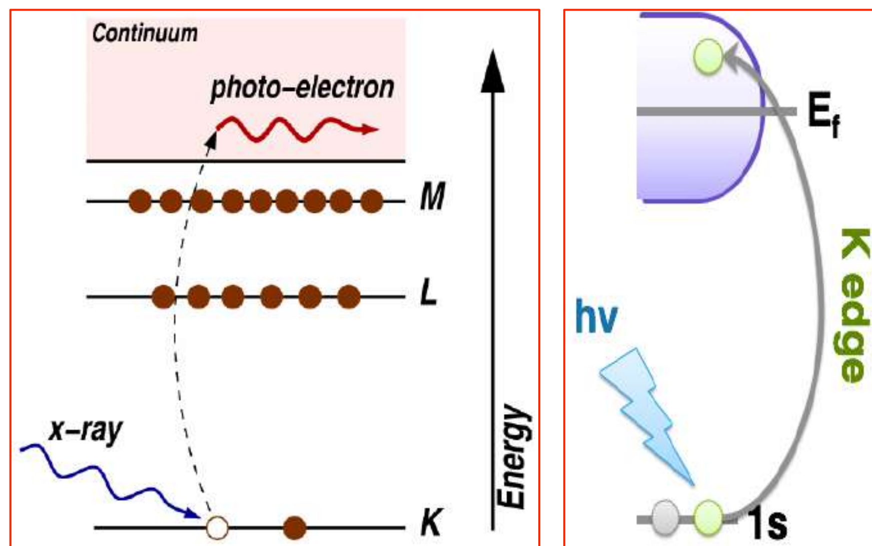


Photons as Ionizing Radiation

- ***Photoelectric effect***
  - Causes ejection of an inner orbital electron and thus also characteristic radiation (energy of fluorescence lines $E_F \approx Z^2$) as orbital hole is filled
  - Energy of ejected photoelectron: $E_e = h\nu - E_B$

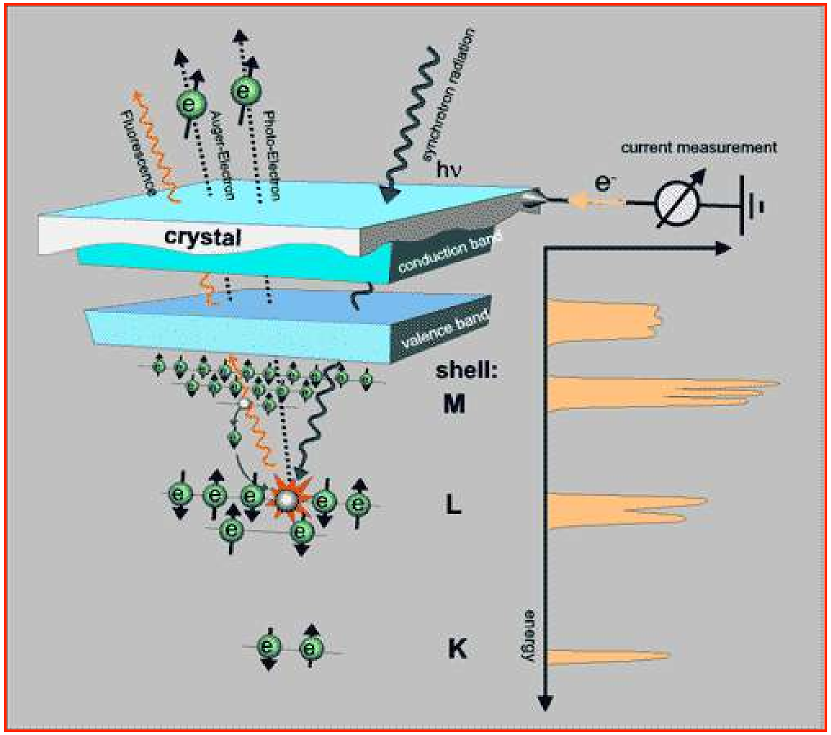


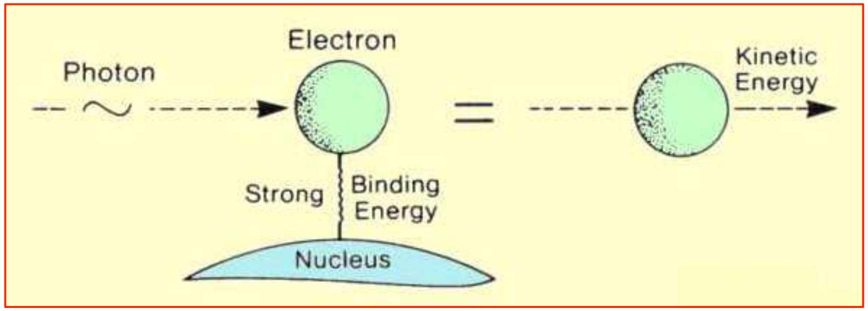
X-ray absorption

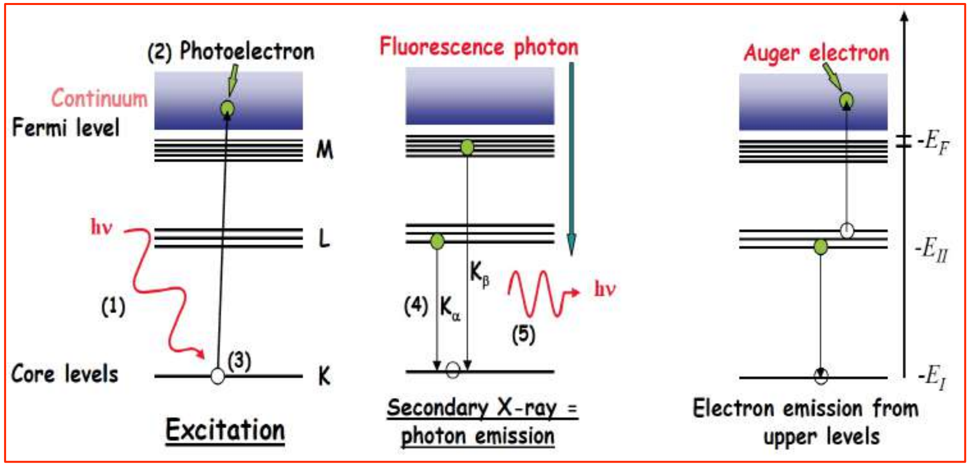


Photoelectric absorption

The probability of a photoelectric interaction is a function of the photon energy and the atomic number of the target atom.
A photoelectric interaction cannot occur unless the incident x-ray has energy equal to or greater than the electron binding energy.

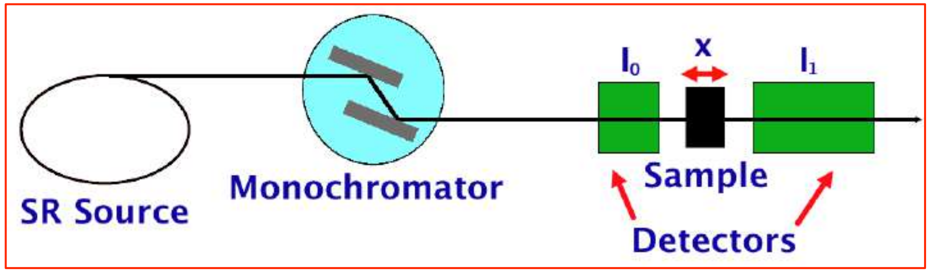






Absorption and decay effects XRF (X Ray Fluorescence) and AES (Auger Electron).

X-ray absorption fine structure spectroscopy - XAFS

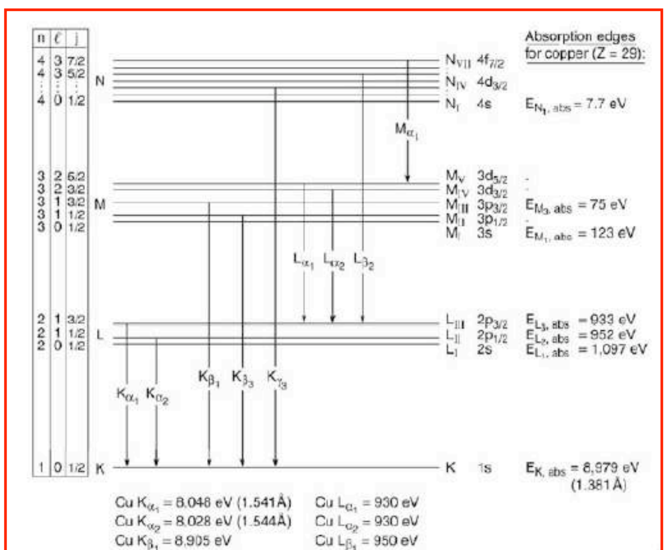


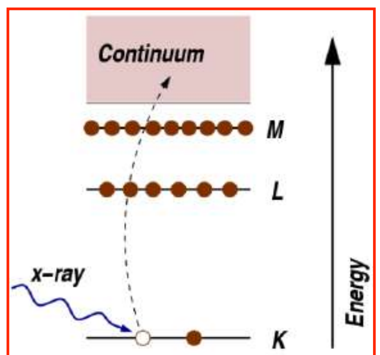
$$I_1 = I_o \exp[-\mu(E)\, x]$$

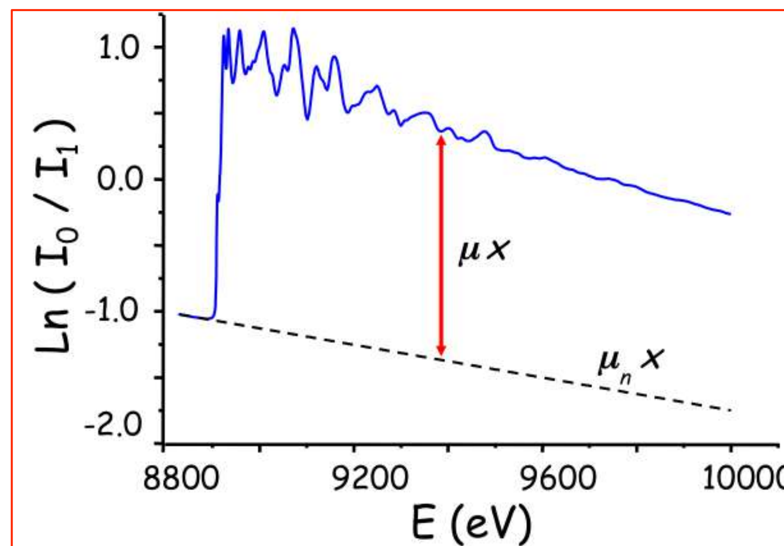
Exponential attenuation or equation of Beer-Lambert

Attenuation coefficient

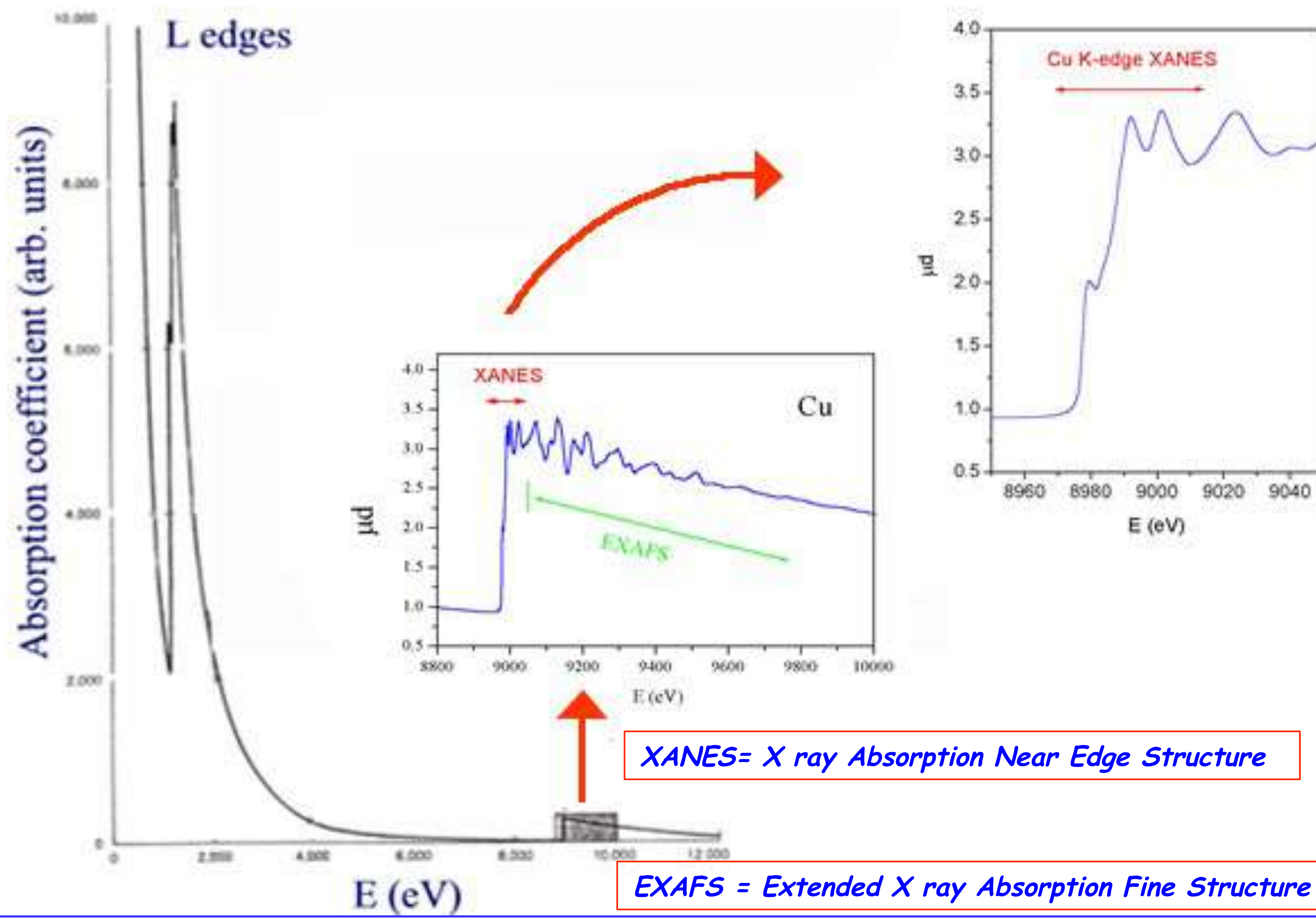
$$\mu(E) = \frac{1}{x} \ln\left(\frac{I_0}{I_1}\right)$$







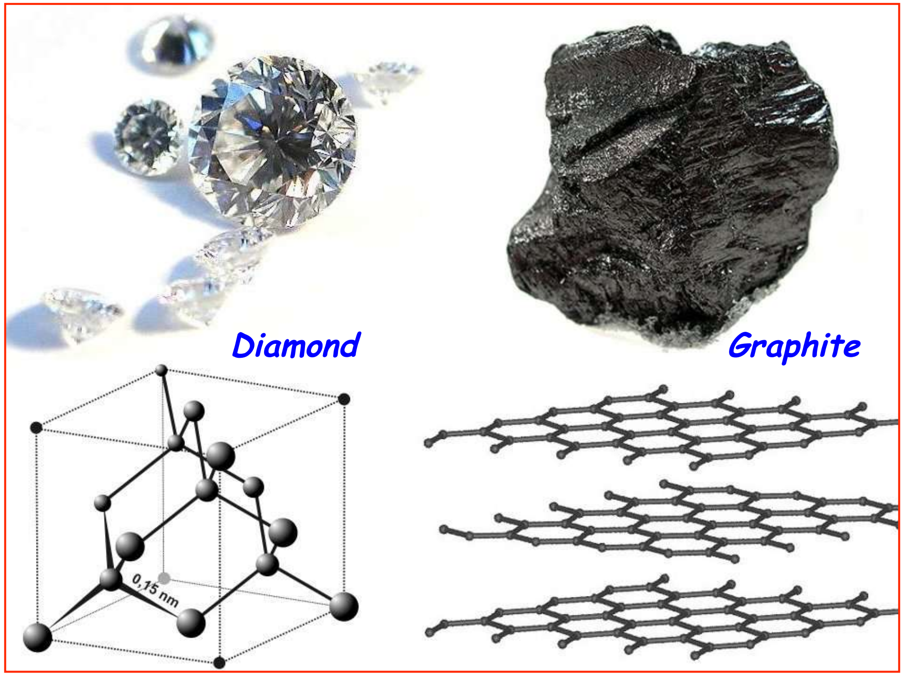
XAFS = XANES + EXAFS



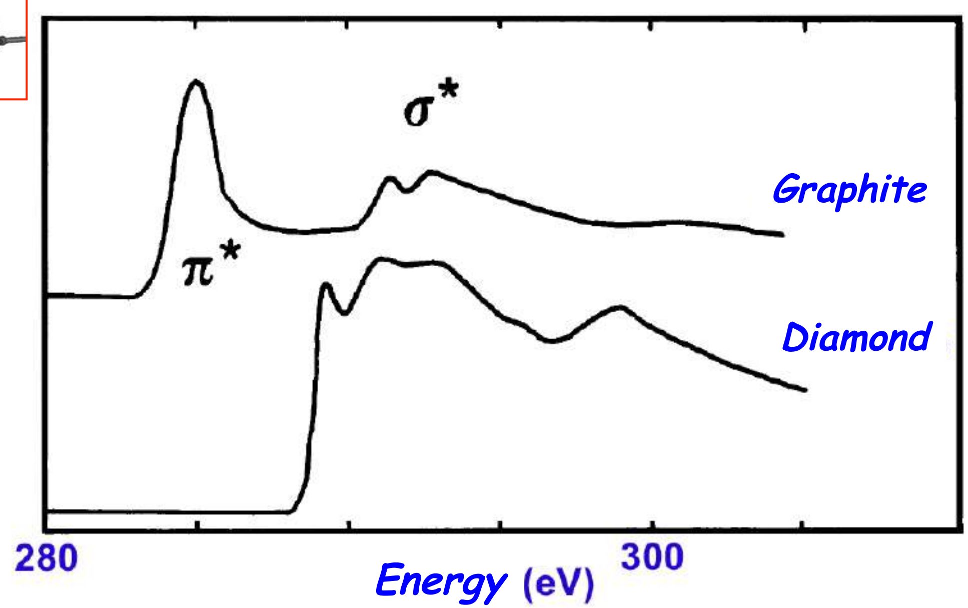
XANES= X ray Absorption Near Edge Structure

EXAFS = Extended X ray Absorption Fine Structure

XANES and Carbon K edge



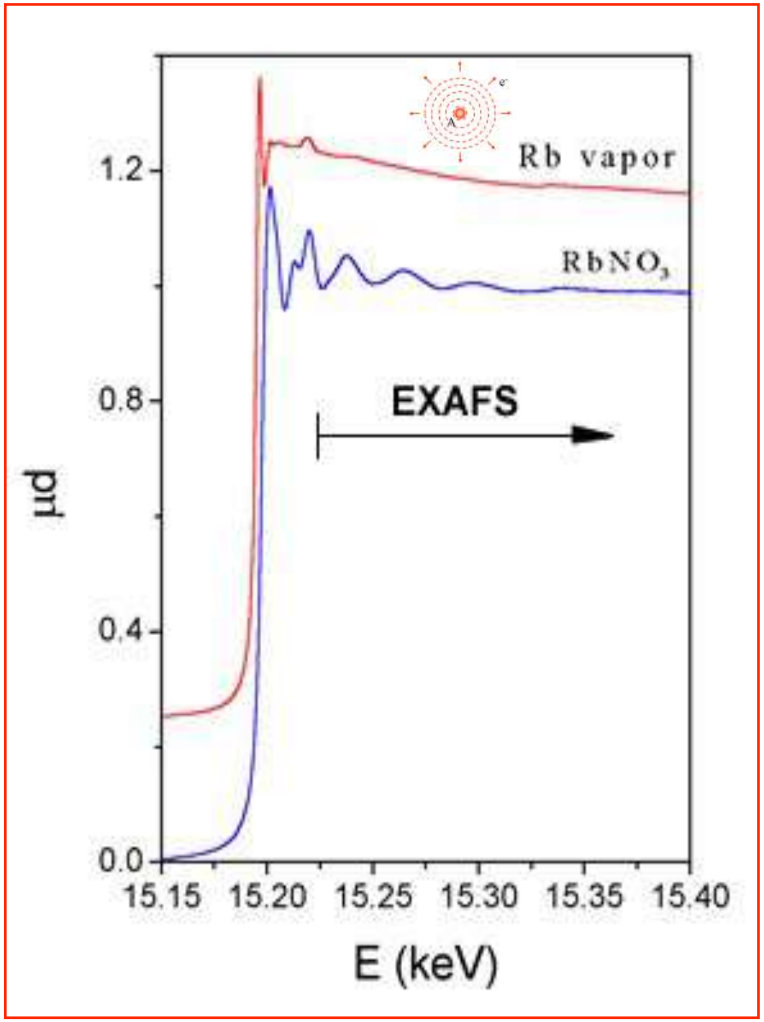
J. Robertson, Prog Solid St. Chem 21, 199 (1991)

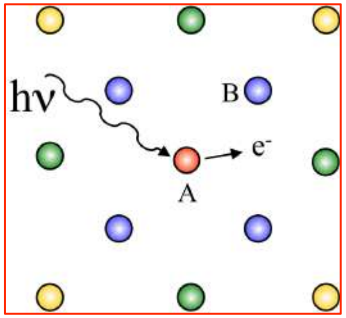


EXAFS

Extended X ray Absorption Fine Structure

EXAFS phenomenological interpretation





X-ray absorption

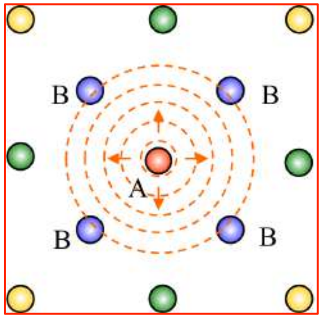
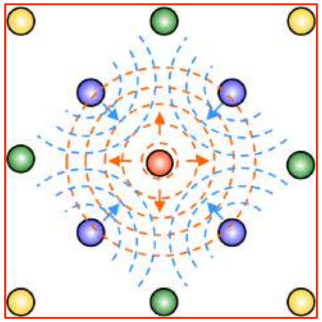
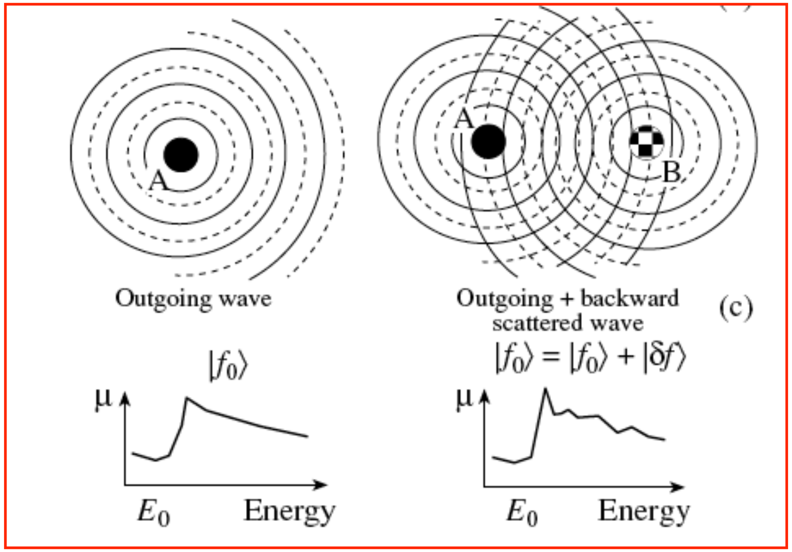


Photo-electron emission

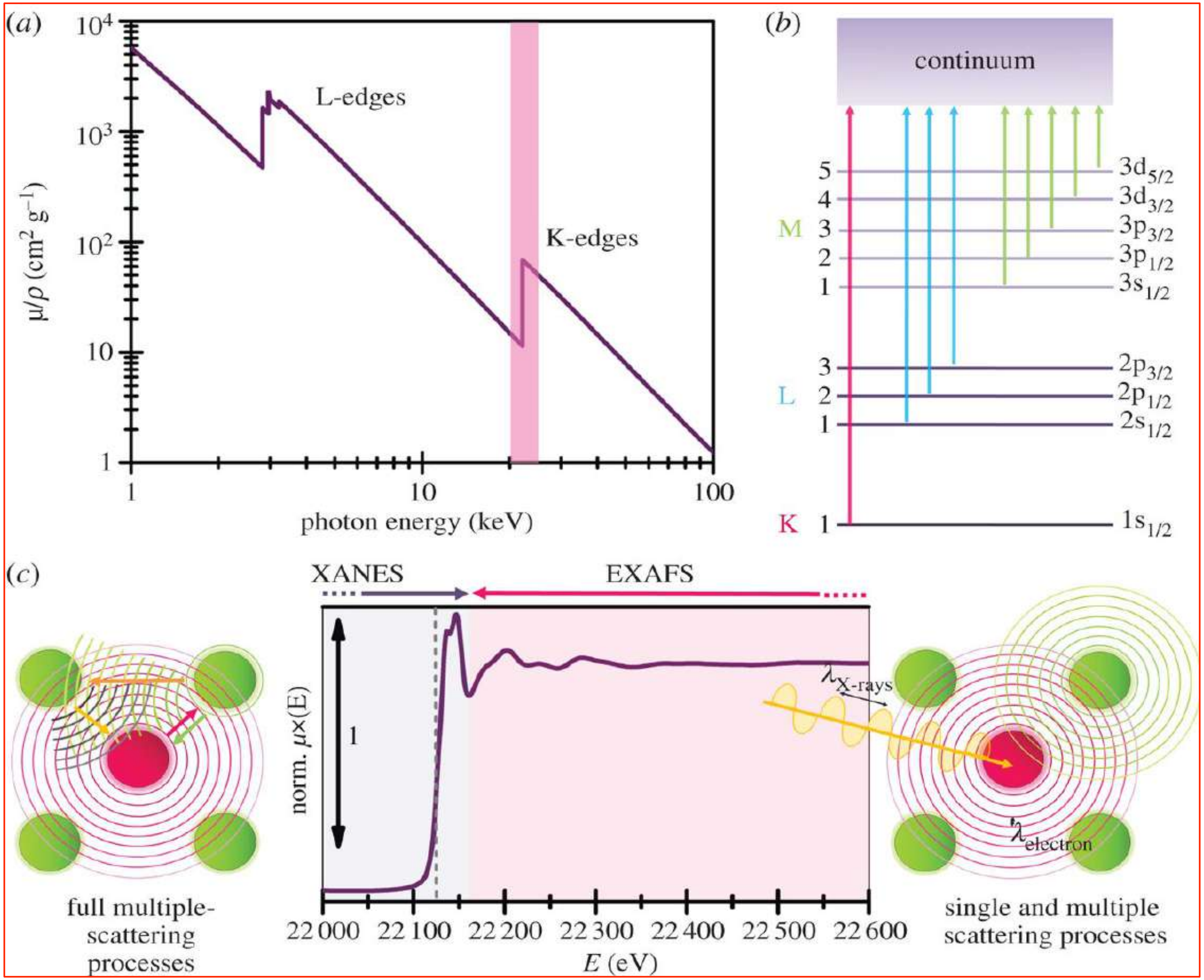


Interference



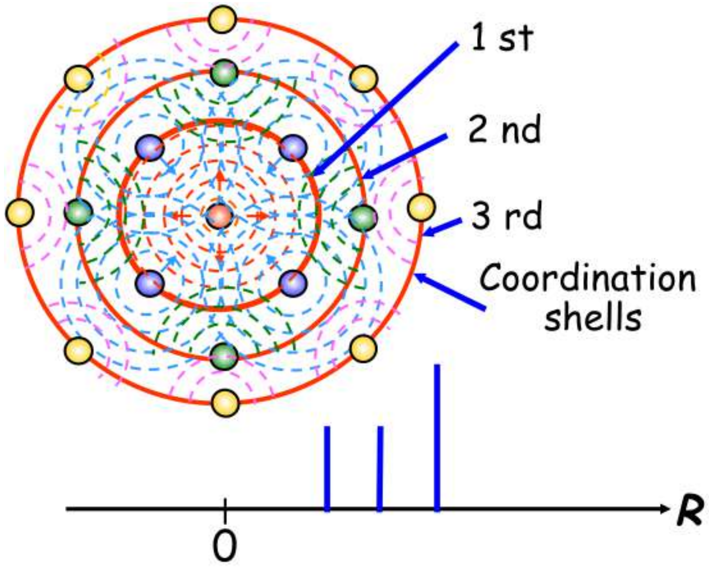
Auto -interference phenomenon of the outgoing photoelectron with its parts that are backscattered by the neighbouring atoms

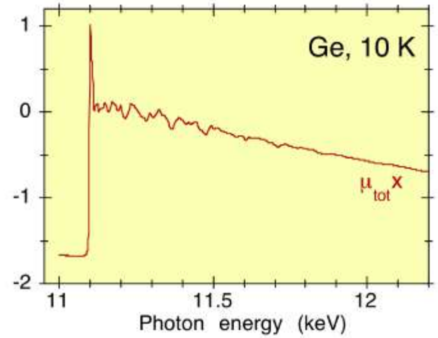
X-ray Absorption

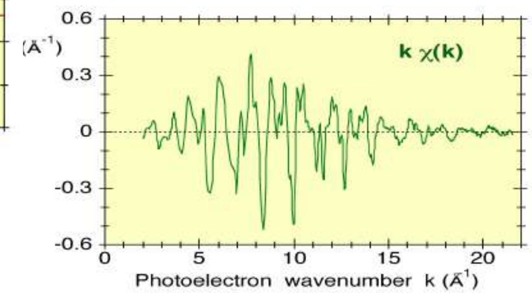


E. Borfecchia et al. - DOI: 10.1098/rsta.2012.0132

EXAFS formula







$$\chi(k) = -\frac{S_0^2}{k}\sum_s N_s \frac{\left|f_s(\pi,k)\right|}{R_s^2} e^{-k^2/\sigma_s^2} e^{-2R_s/\lambda_s} \sin\left(2kR_s + \phi_s(k)\right)$$

Coordination number

Debye Waller factor

Interatomic distance

$$k = \sqrt{\frac{2m}{\hbar^2}\left(E - E_0\right)}$$

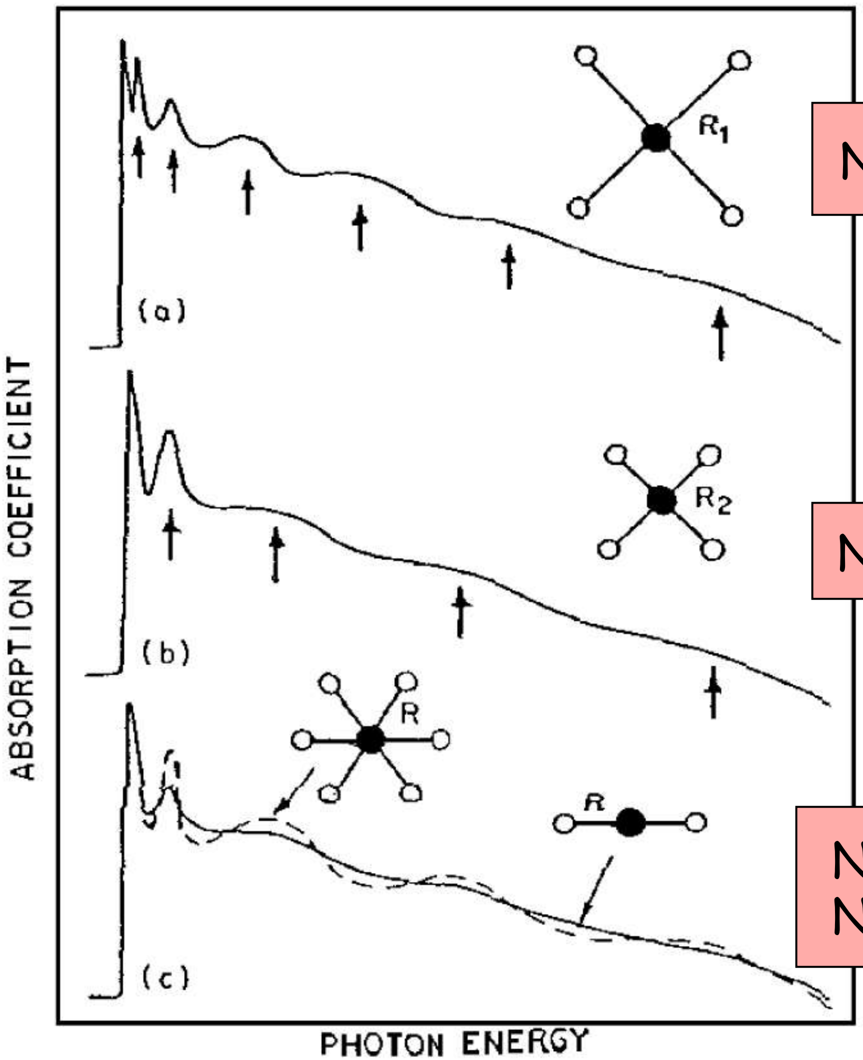
k = wavenumber

Thermal disorder: e^{-k^2/σ^2}

Electron mean free path: λ

Inelastic scattering effect: S_0^2

EXAFS



N=4 $R=R_1$

N=4 $R=R_2$

N=6 R=R
N=2 R=R

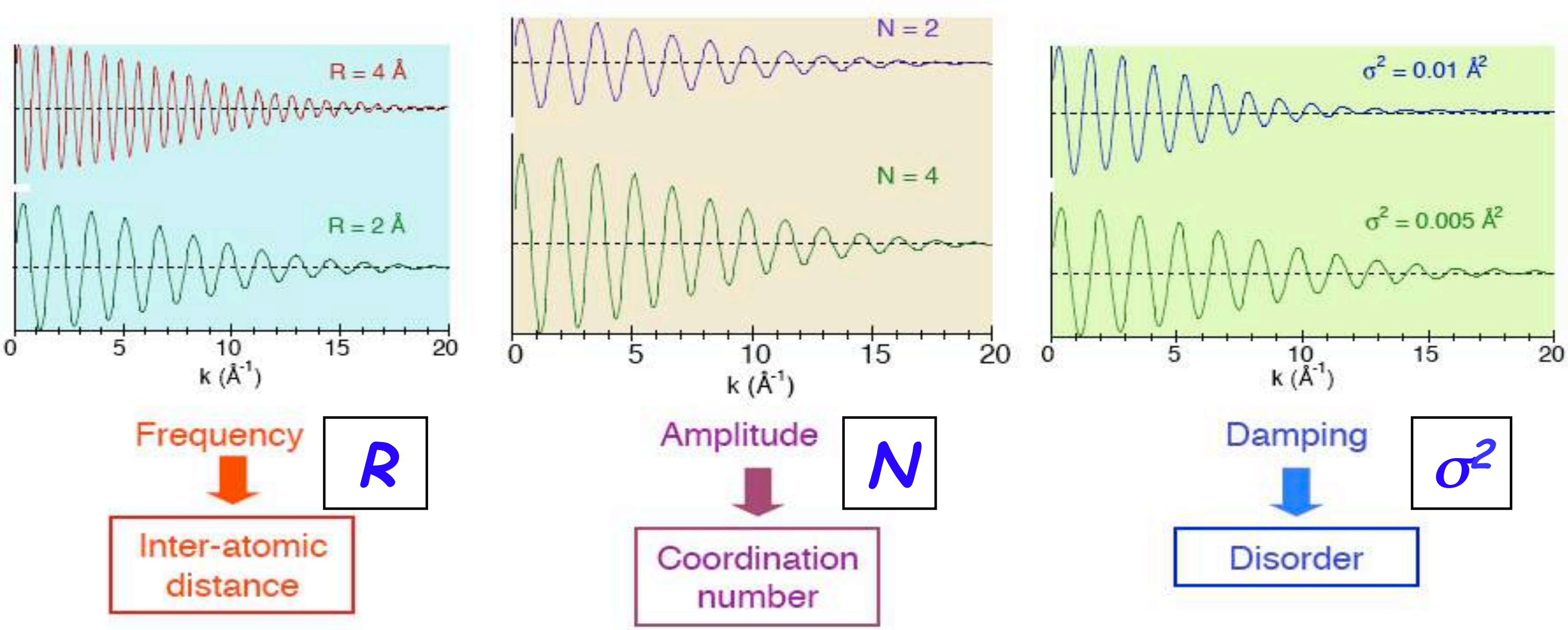
EXAFS and structural information

$$\chi(k) = -\frac{S_0^2}{k}\sum_s N_s \frac{\left|f_s(\pi,k)\right|}{R_s^2} e^{-k^2/\sigma_s^2} e^{-2R_s/\lambda_s} \sin\left(2kR_s + \phi_s(k)\right)$$

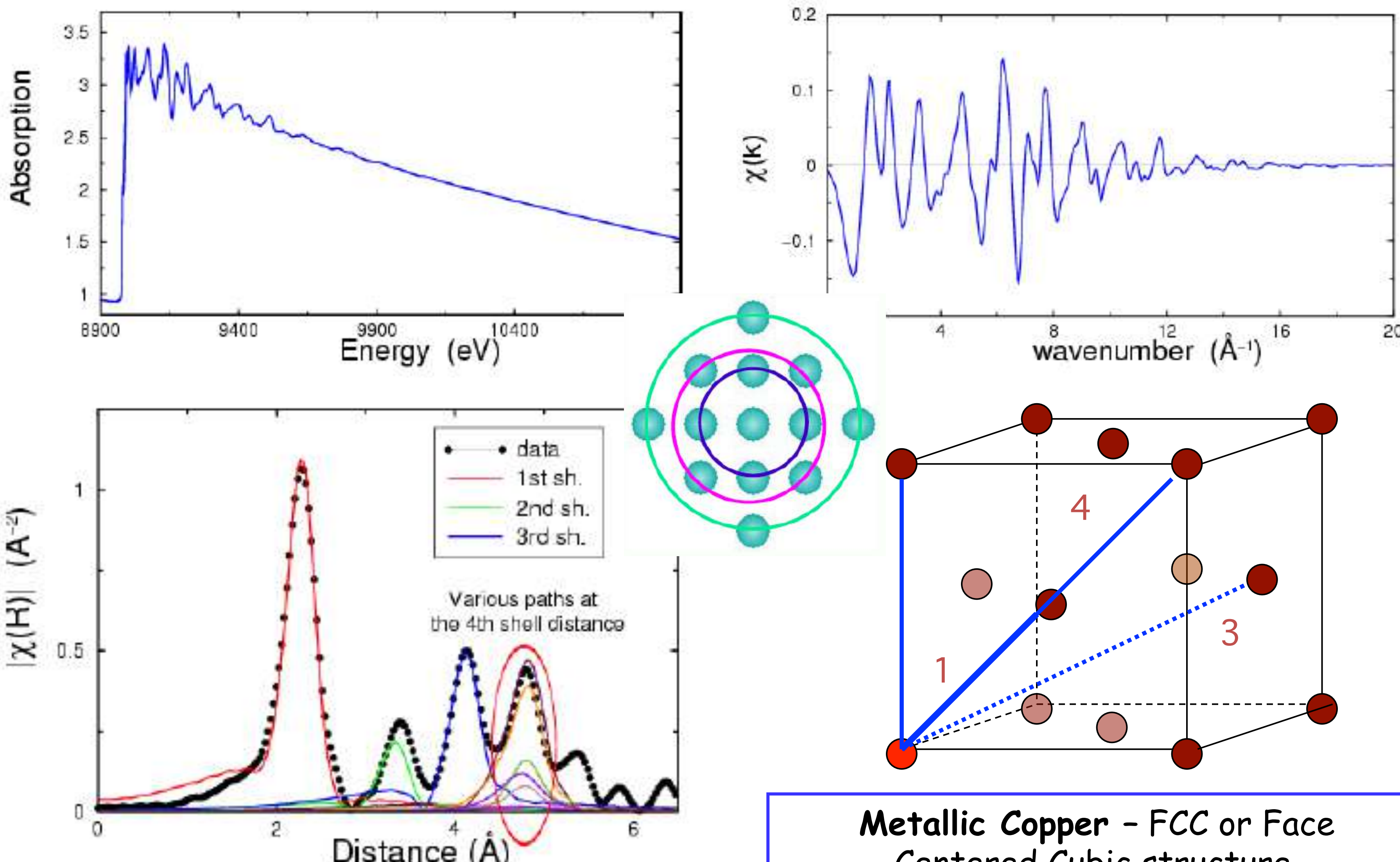
Coordination number

Debye Waller factor

Interatomic distance

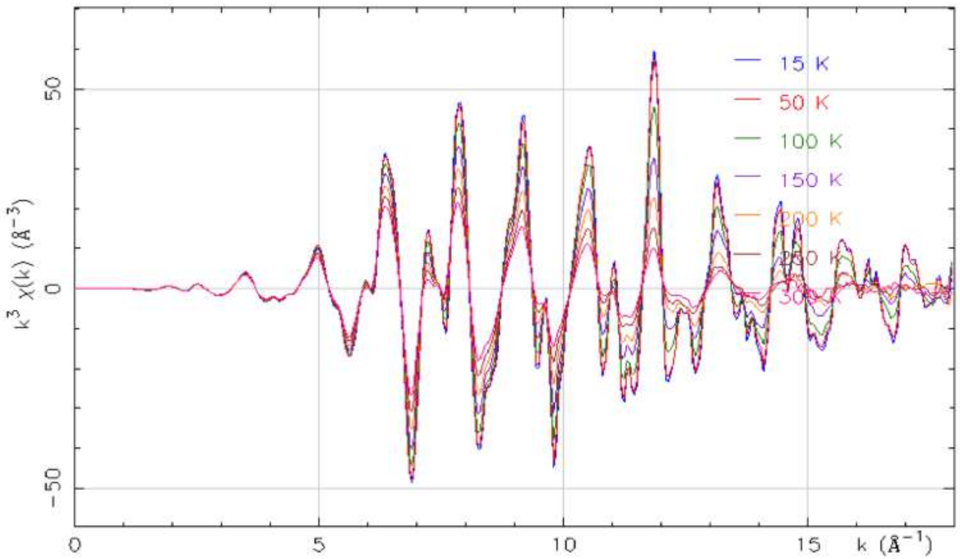


EXAFS data analysis



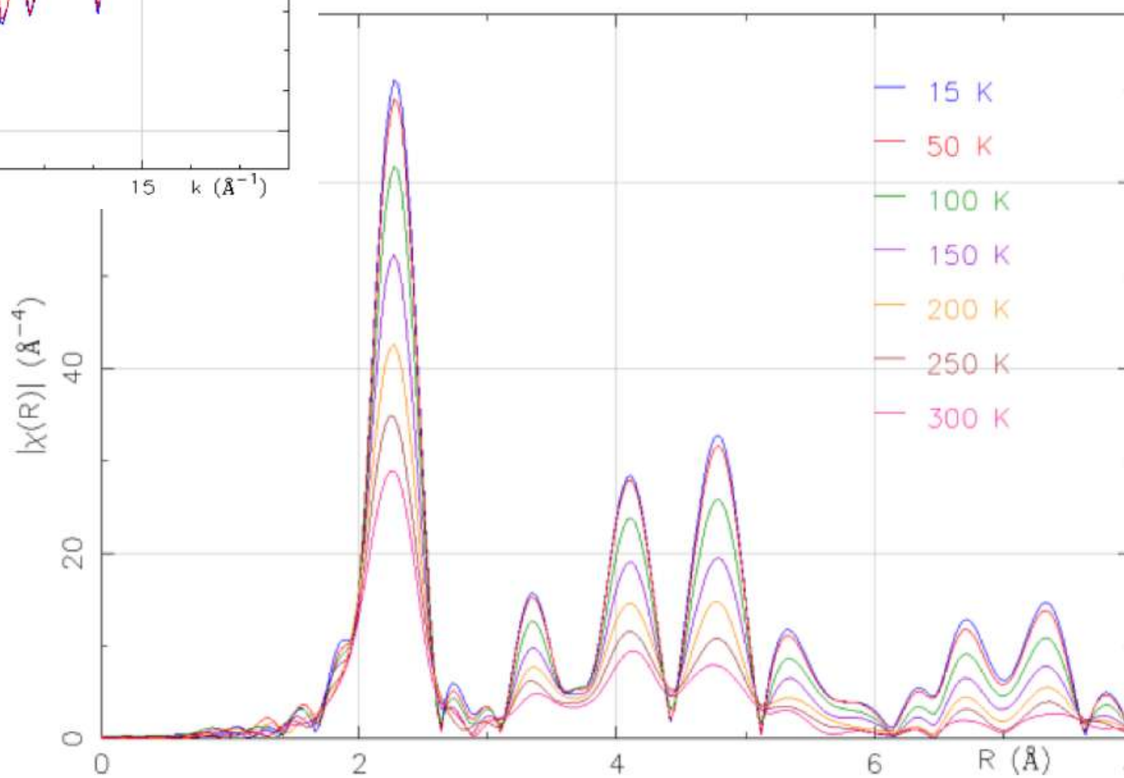
Metallic Copper – FCC or Face Centered Cubic structure.

Cu foil and temperature effects



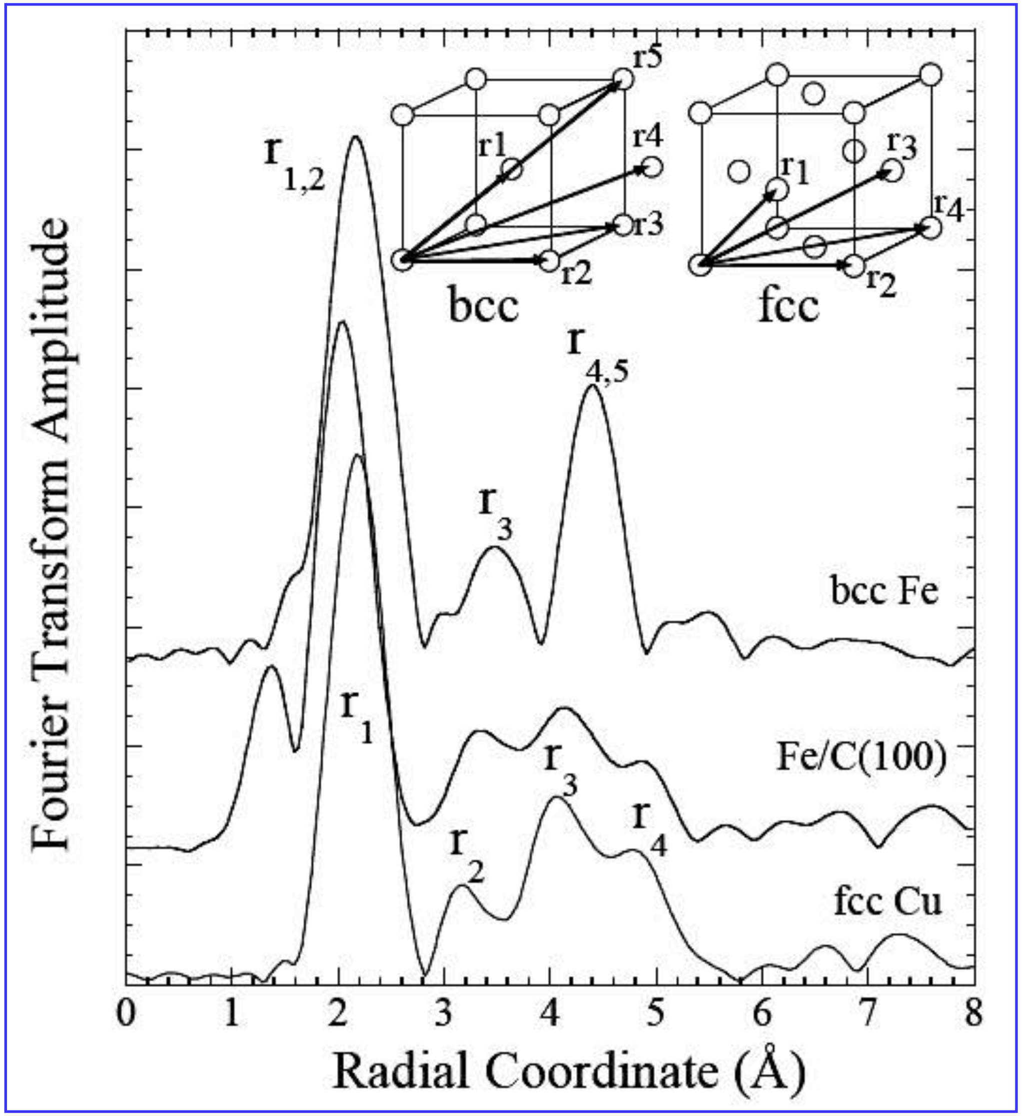
EXAFS spectra as a function of temperature.

Thermal disorder: e^{-k^2/σ^2}



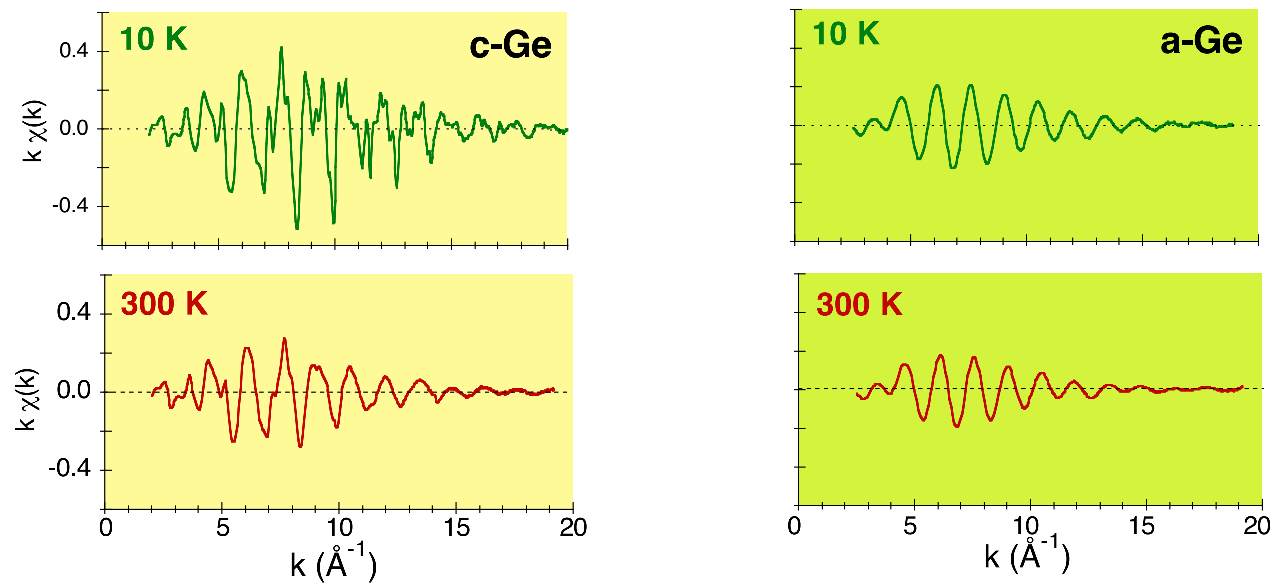
Fourier transforms of the EXAFS spectra.

EXAFS data analysis

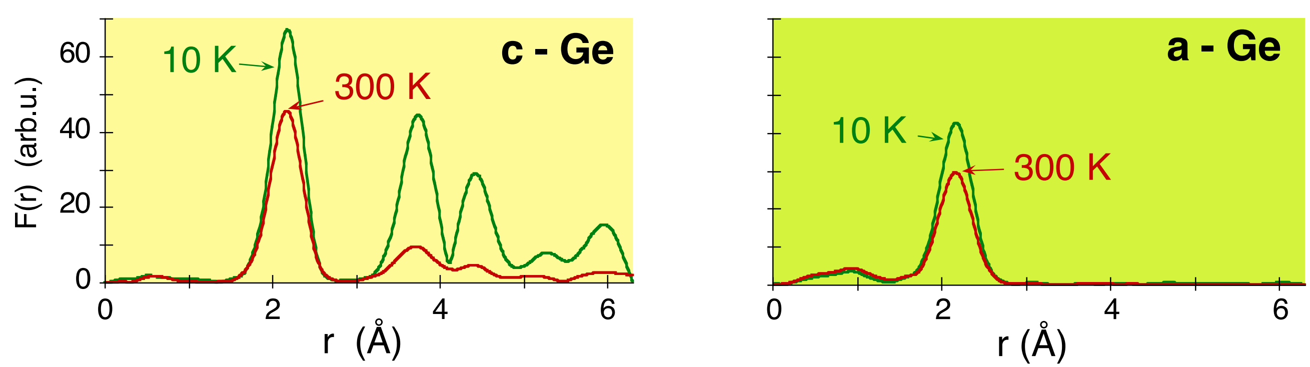


EXAFS data analysis

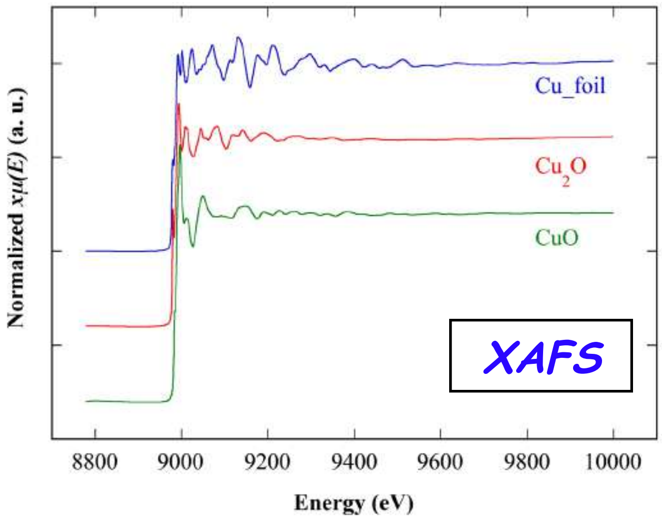
EXAFS signals

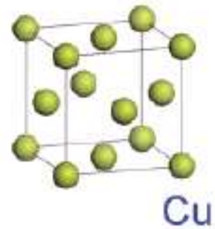


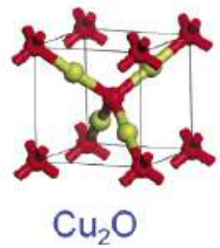
Fourier transforms

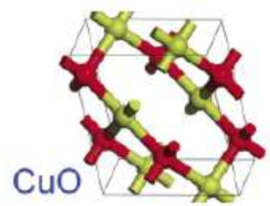


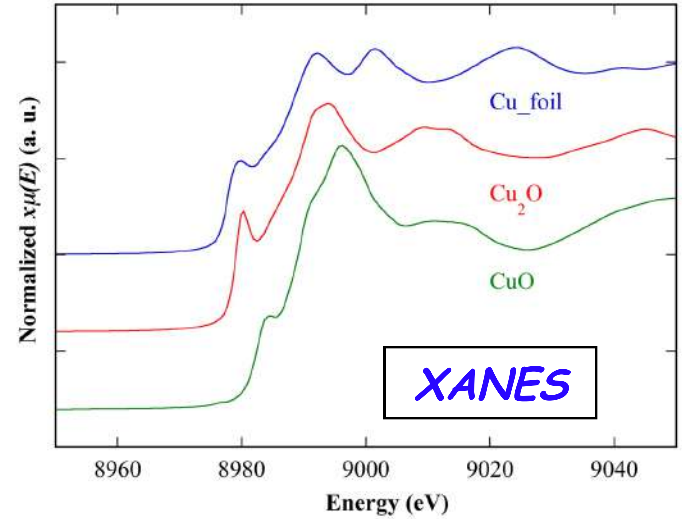
Cu Cu_2O CuO

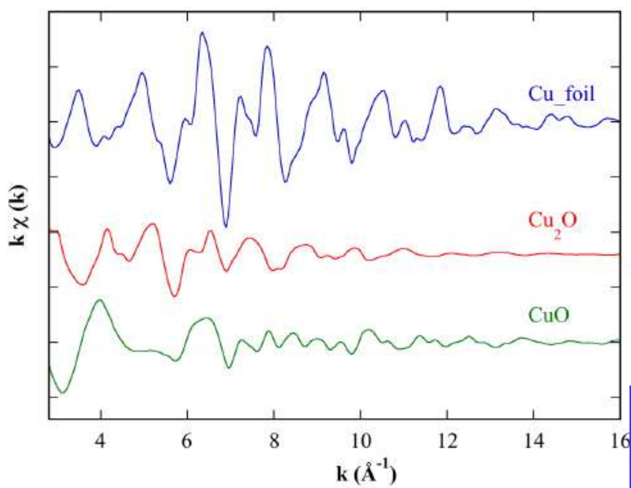








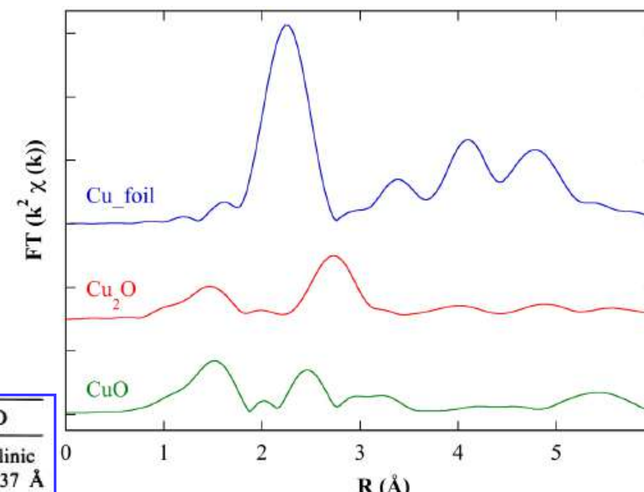




EXAFS

Cu metal FCC a= 3.61Å

	Cu_2O	CuO
Lattice parameter	Cubic $a = 4.27$ Å	Monoclinic $a = 4.6837$ Å $b = 3.4226$ Å $c = 5.1288$ Å $\beta = 99.54°$
Shortest distances		
$d_{Cu\text{-}O}$	1.84 Å	1.95 Å
$d_{O\text{-}O}$	3.68 Å	2.62 Å
$d_{Cu\text{-}Cu}$	3.02 Å	2.90 Å

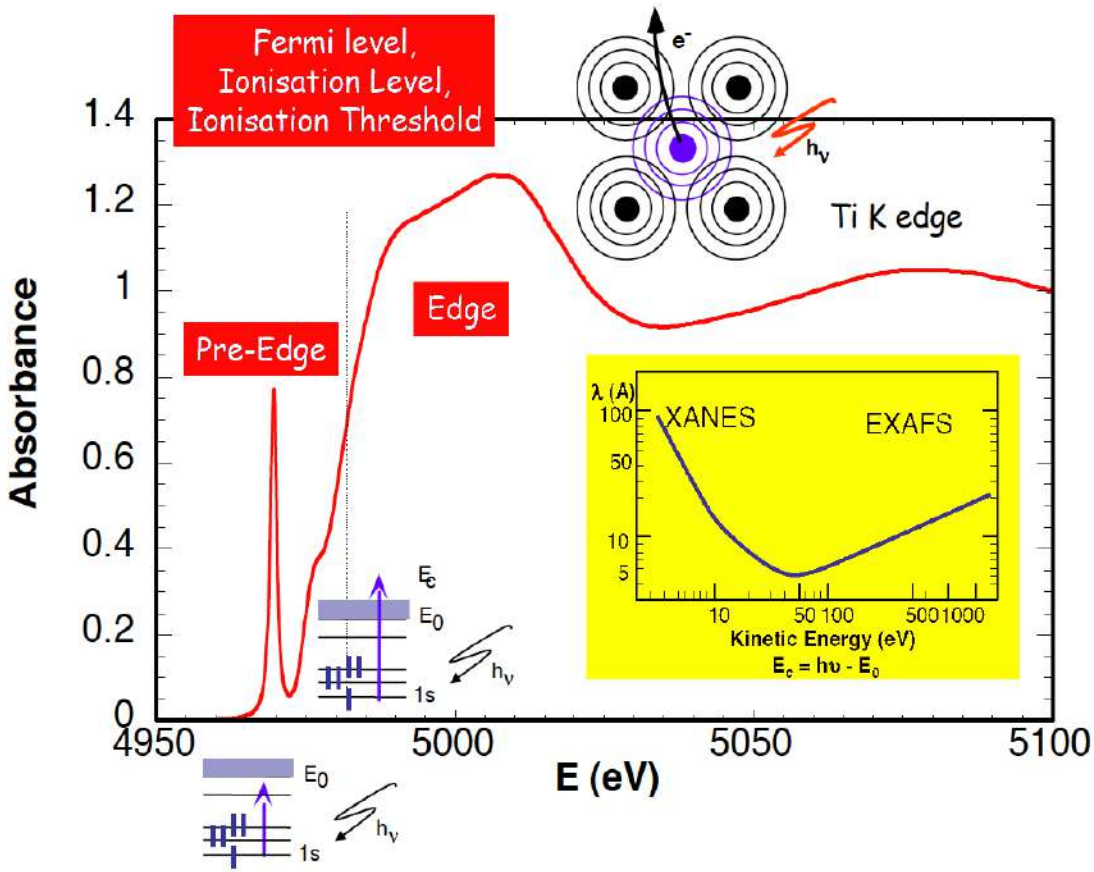


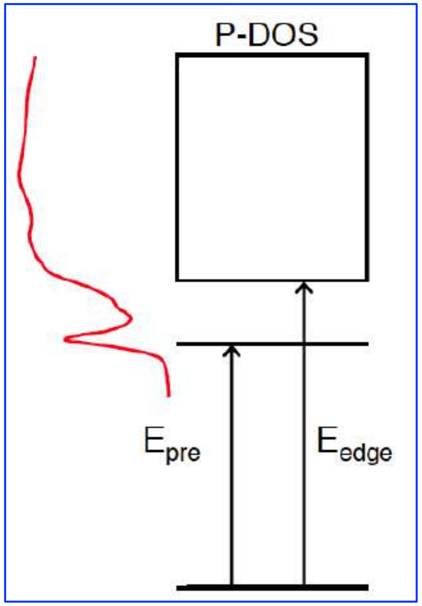
Fourier Transform

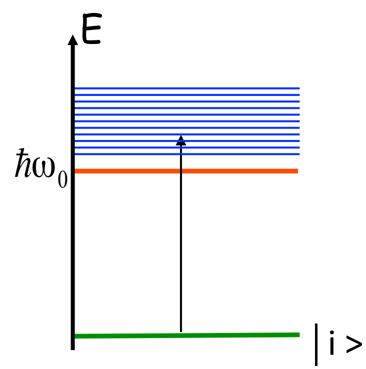
XANES

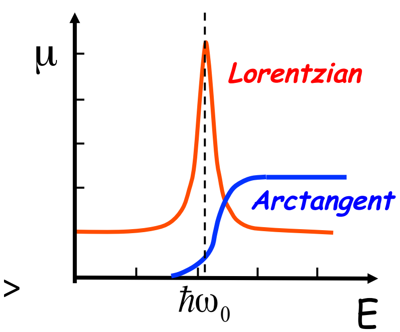
X ray Absorption Near Edge Structure

XANES



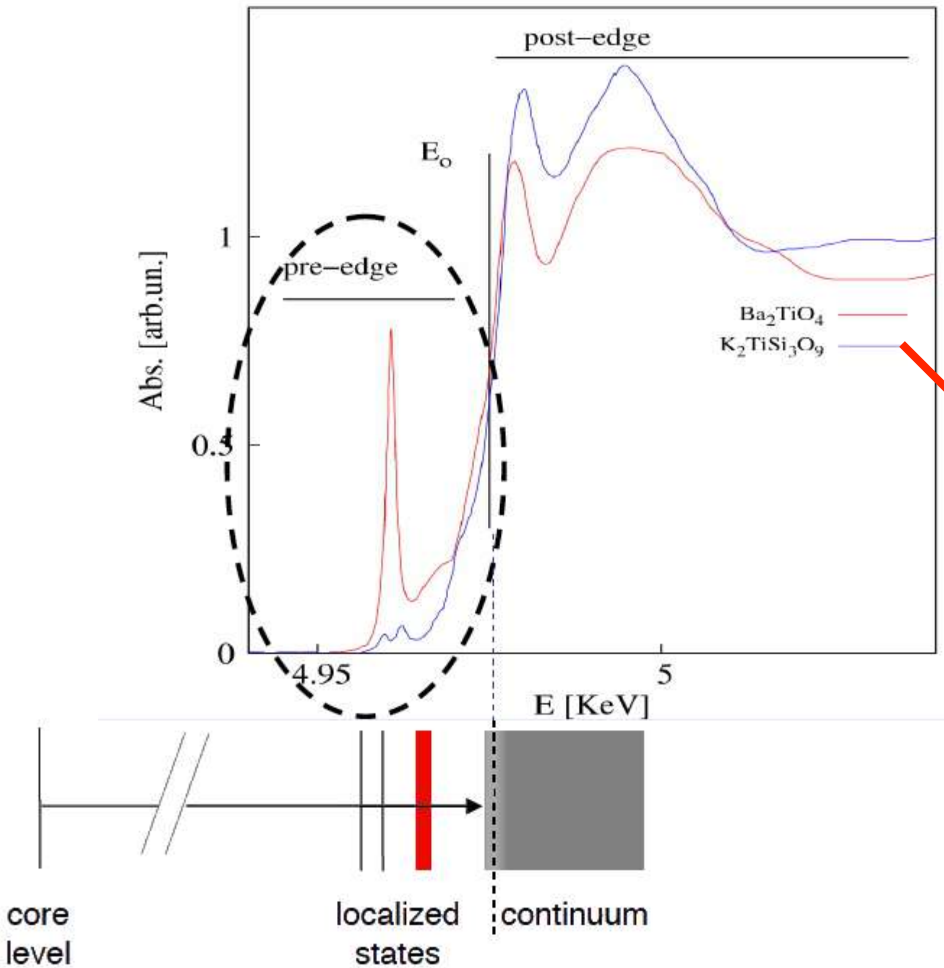


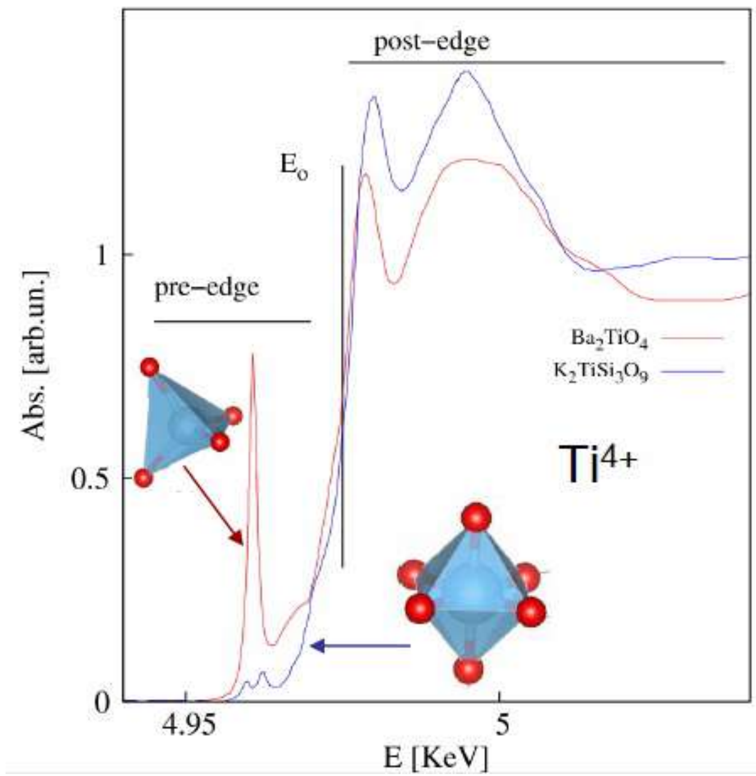




The local symmetry around the absorbing atom (symmetry, distance ligand-metal), the electronic structure of the absorbing atom (electronic filling of the valence state, oxidation state, spin state…)

Pre-edge region



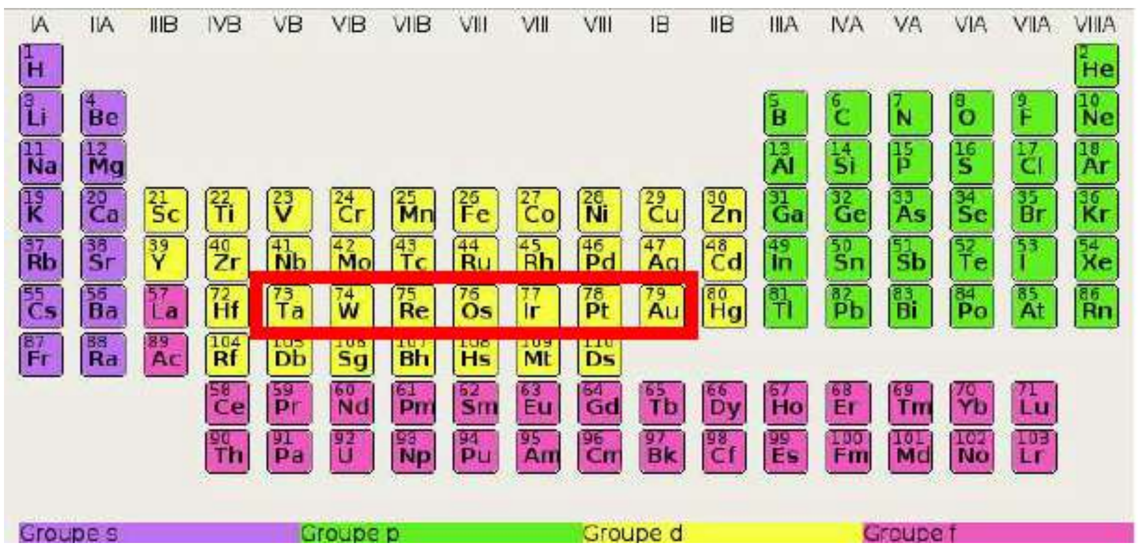


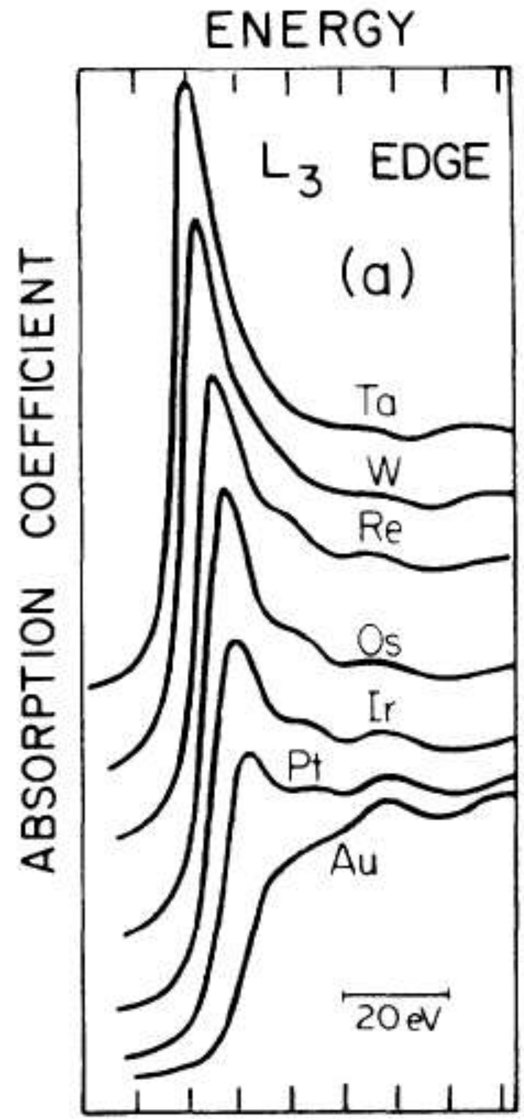
Pre-edge peaks are due to electronic transitions (mainly dipole allowed) to empty bound states near the Fermi level.

The peak due to s --> p transitions (K edge) provides information on the absorber local geometry. In the Tetrahedral case (not centrosymmetric like Oh case) the p - d mixing is allowed and this gives the largest pre-edge peak.

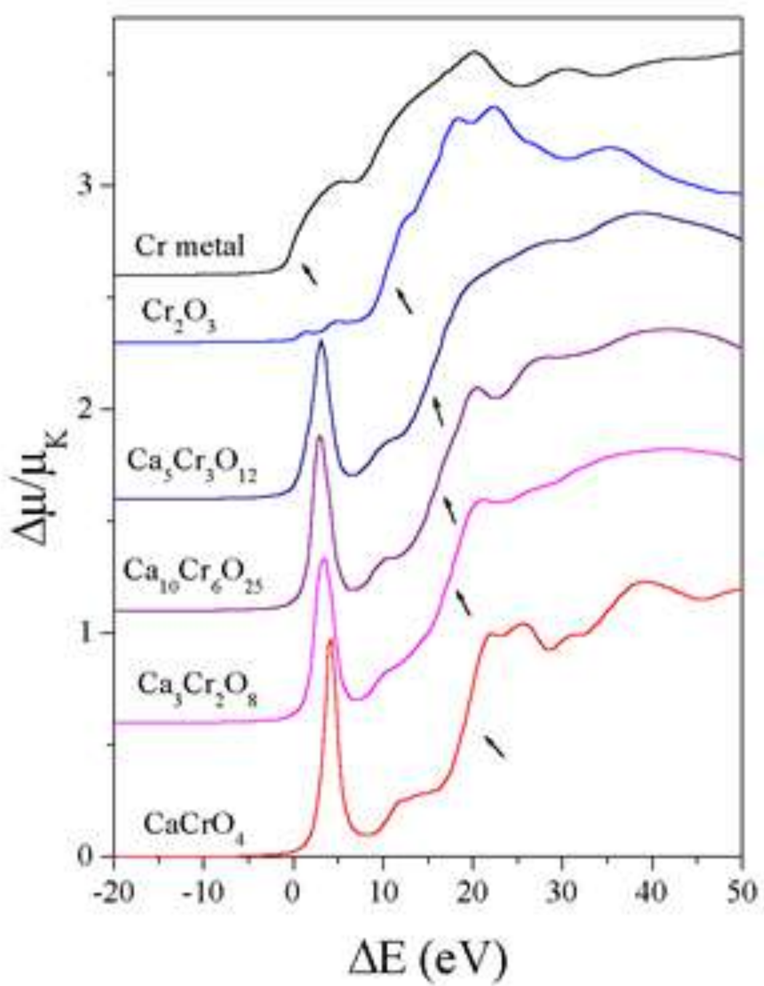
Shape of whitelines and L-edges

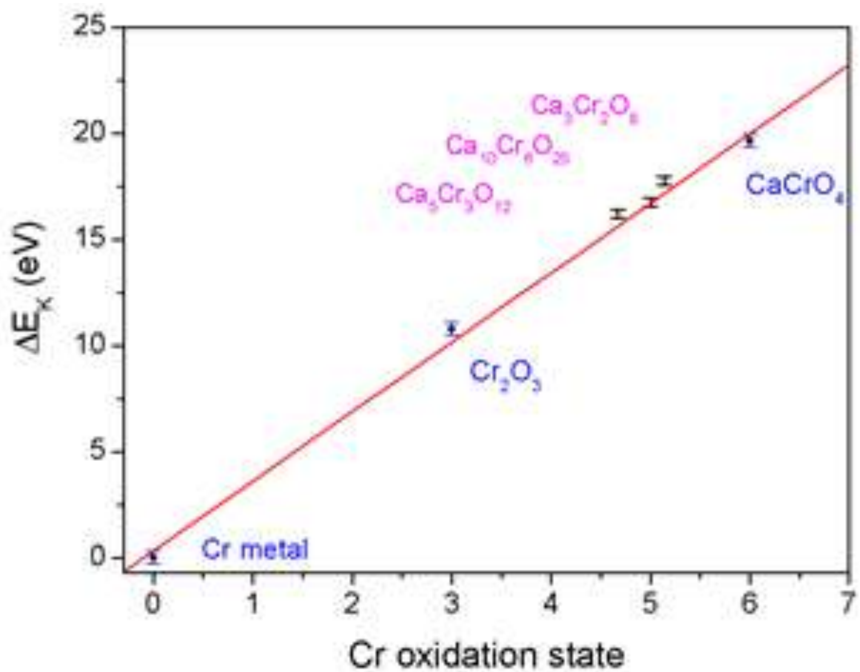
Whitelines present in the L-edges of atoms with 4d and 5d electrons, reflect holes in d-bands: the intensity decreases as a function of the increasing number of electrons in the d-band. In Au the 5d band is full.
Phys. Rev. B 36 (1987) 2972





XANES and oxidation state

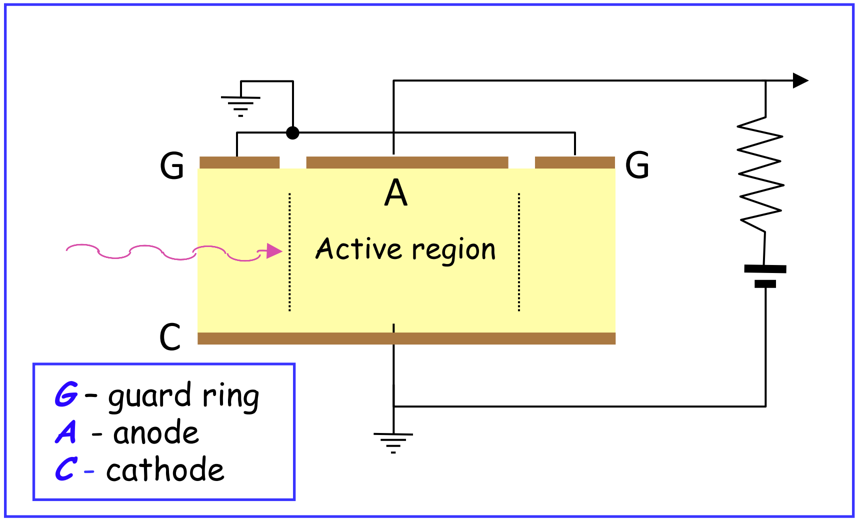


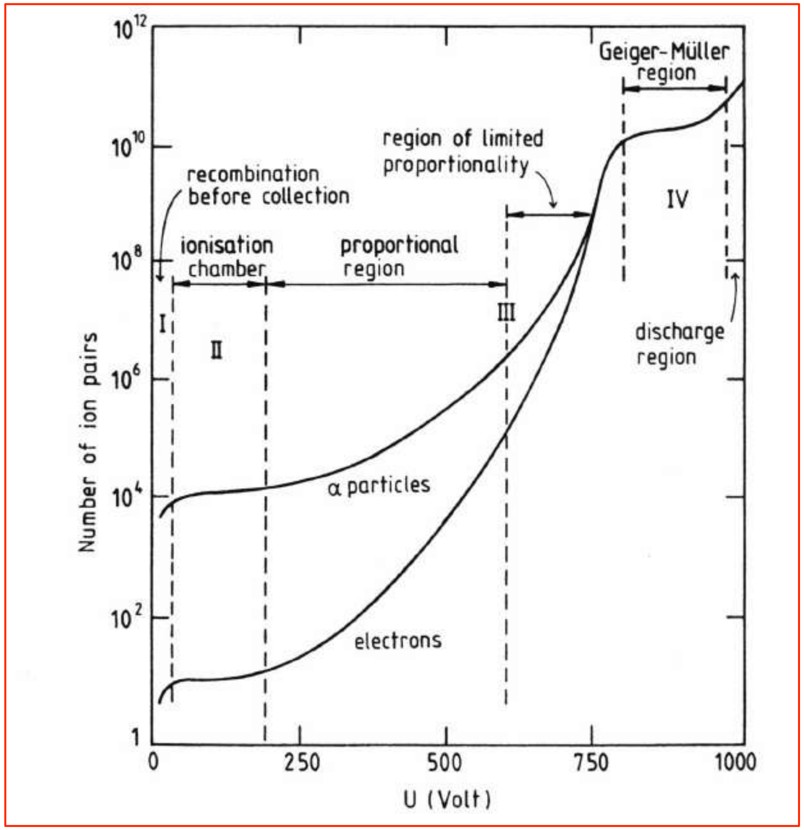


The edge, E_0 (arrow), defines the onset of continuous states (this is not not the Fermi level).
E_0 is a function of the absorber oxidation state and geometry. It may also increase by several eV due to oxidation.

Detectors and
Gas ionization chambers

X-ray Ion Chamber

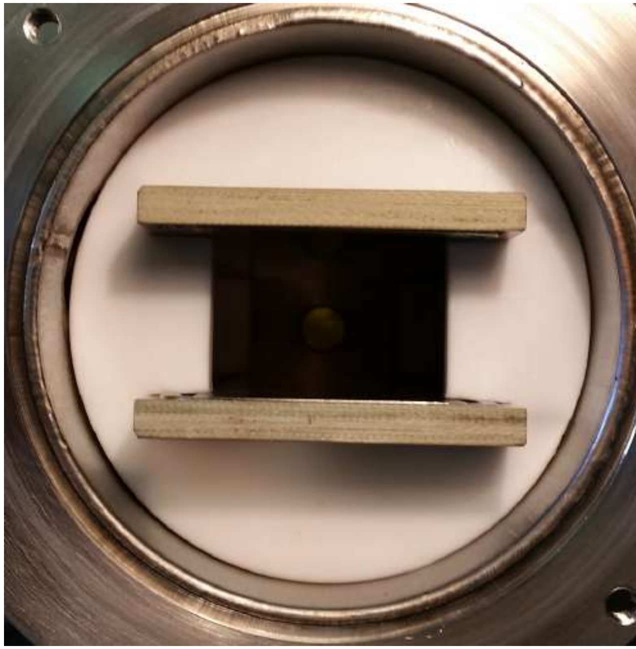




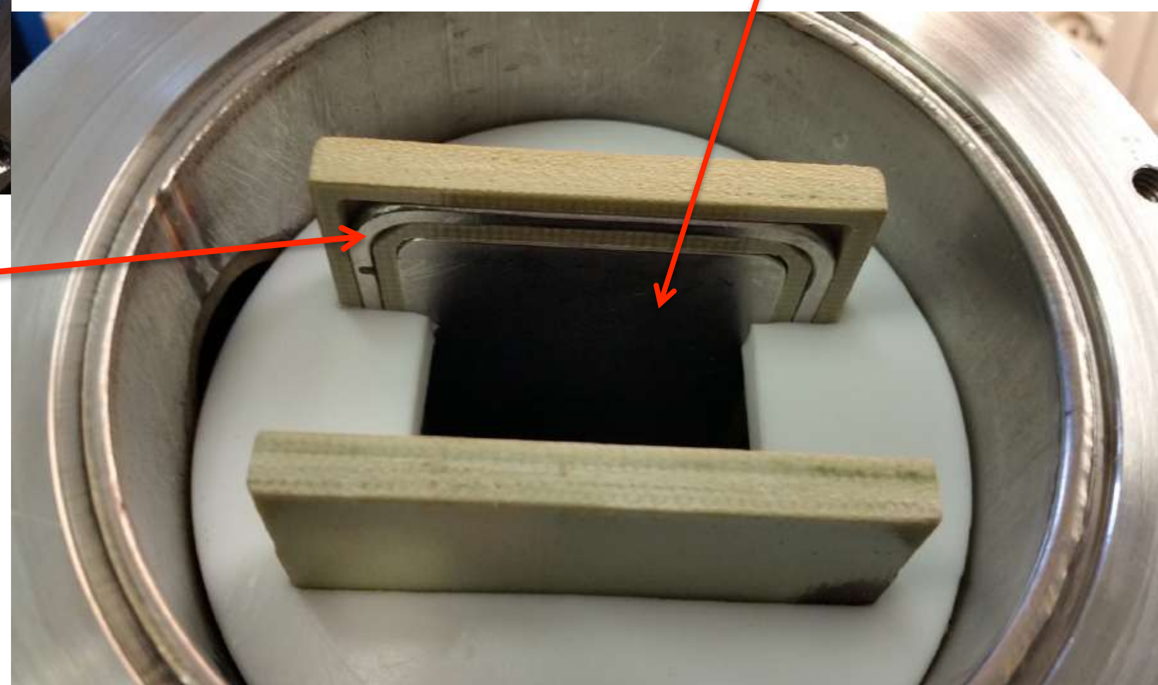
Gas ionization detectors are commonly used as integrating detectors to measure beam flux rather than individual photons. A typical detector consists of a rectangular gas cell with thin entrance and exit windows.

Inside the detector, an electric field is applied across two parallel plates. Some of the x-rays in the beam interact with the chamber gas to produce fast photoelectrons, Auger electrons, and/or fluorescence photons. The energetic electrons produce additional electron-ion pairs by inelastic collisions, and the photons either escape or are photo-electrically absorbed. The electrons and ions are collected at the plates, and the current is measured with a low-noise current amplifier. The efficiency of the detector can be calculated from the active length of the chamber, the properties of the gas, and the x-ray absorption cross section at the appropriate photon energy.

X-ray Ion chamber



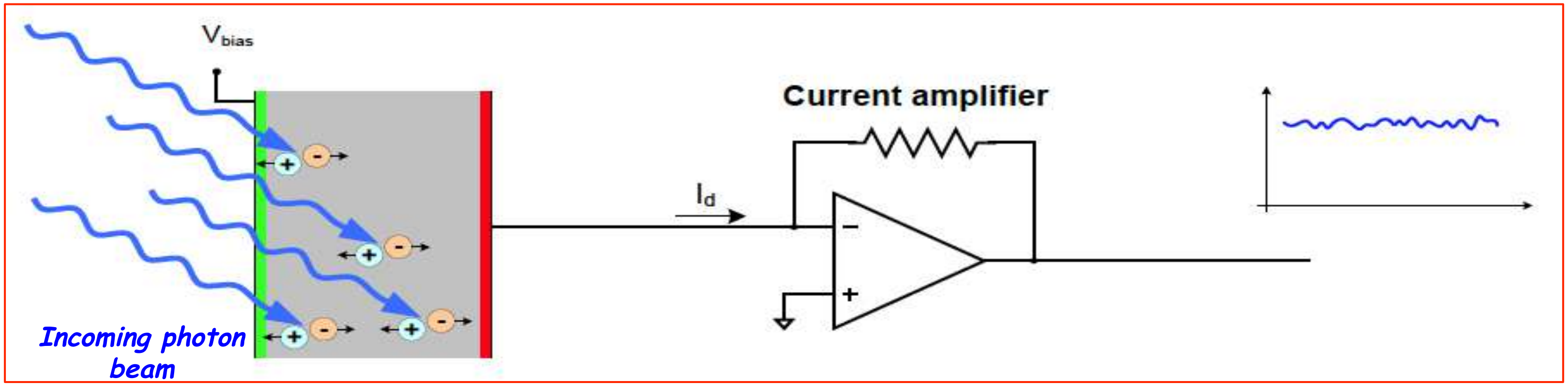
Ion chamber with parallel plates.



Guard ring

In the parallel plate chamber the charge-collecting electrode is surrounded by an annular ring. The annular ring represents the guard ring (or guard electrode) and is separated from the collecting electrode by a narrow insulating gap, and the applied voltage to the guard ring is the same as that to the collecting electrode.

Direct detection: charge conversion scheme and intensity measurement

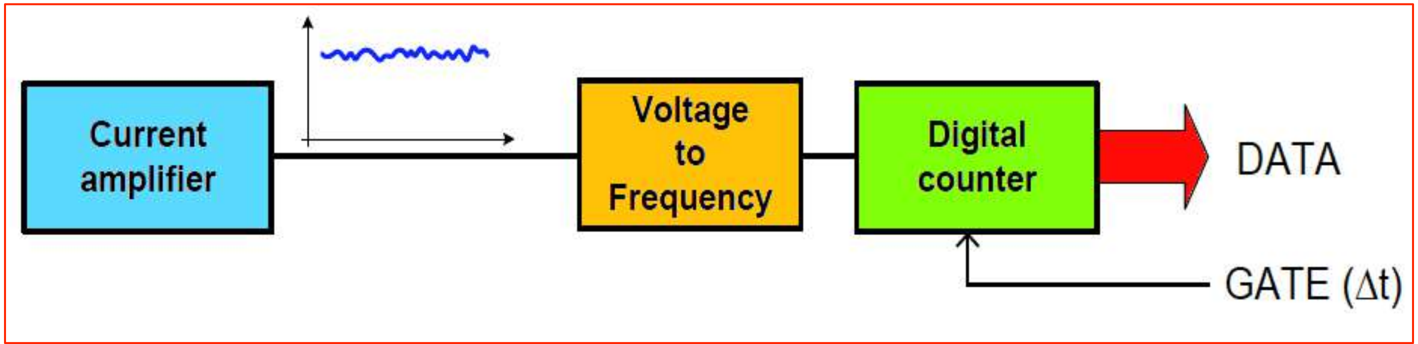


The measured intensity is usually integrated during a well defined time interval and is proportional to the number of incident X-ray photons (N_{ph}).

Intrinsic statistical noise (Poisson statistics): $\sigma_{N_{ph}} = \sqrt{N_{ph}}$ Effective: $\sigma_{N_{ph}} = \sqrt{FN_{ph}}$

Fano factor F accounts empirically for deviation from Poisson statistics F ≈ 0.2 for gasses, ≈ 0.1 for semiconductors

The measured intensity is integrated during the exposure time Δt.

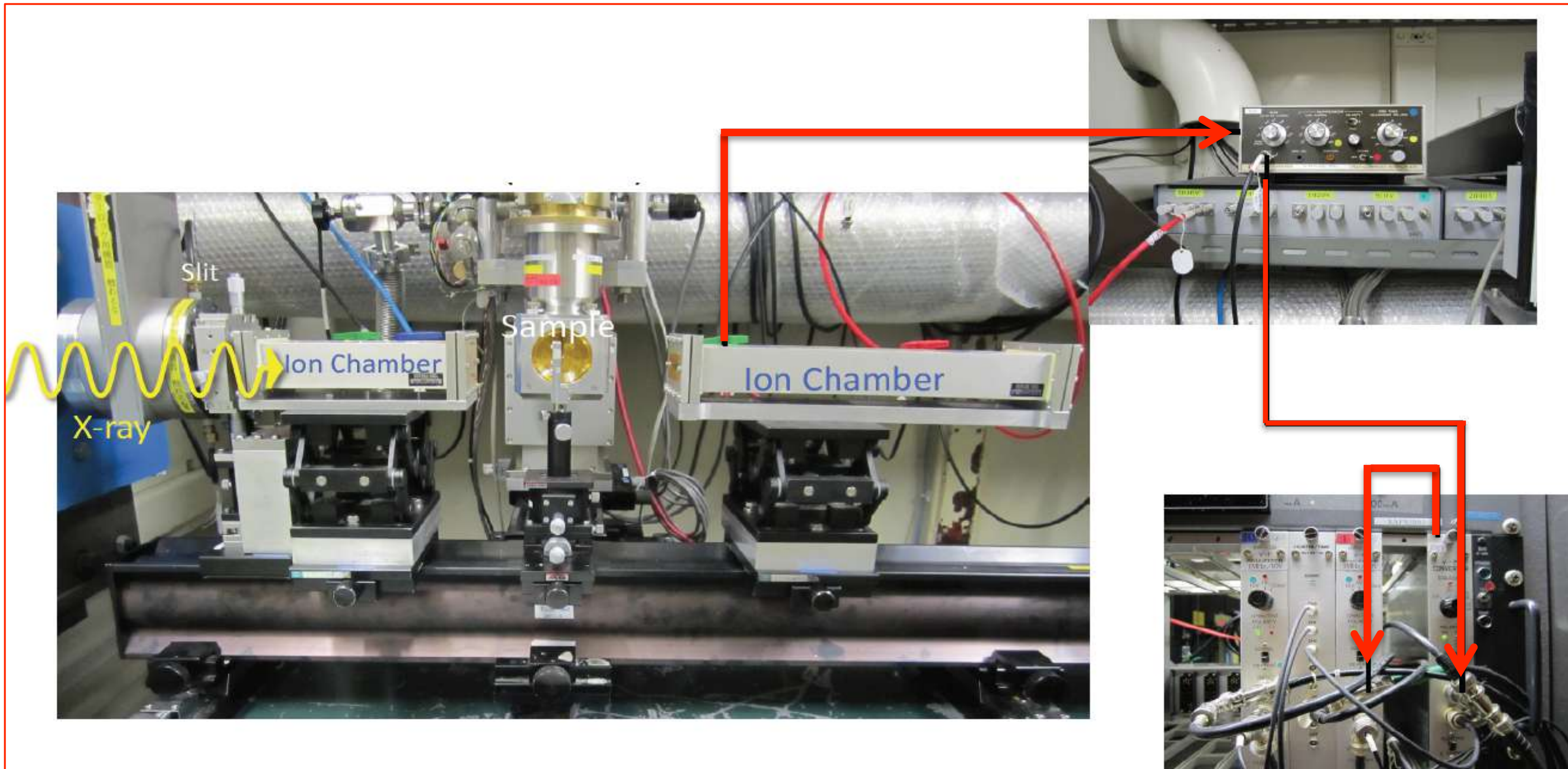


Setup: XAFS in transmission mode

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

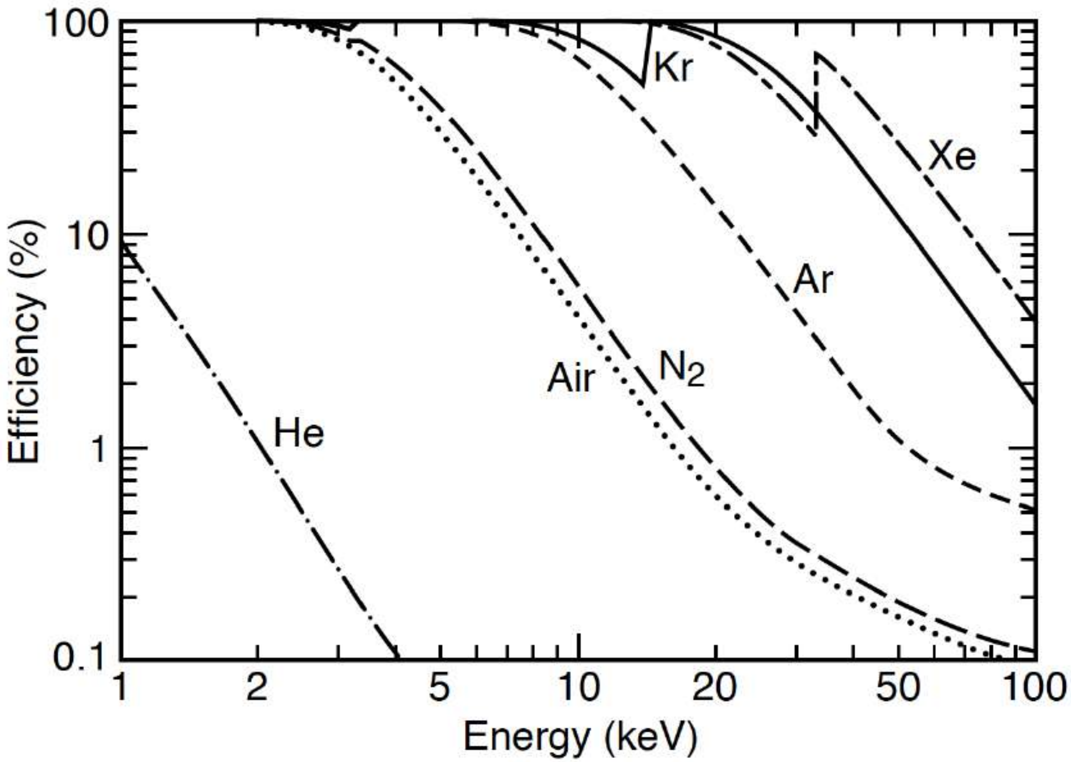
Current proportional to the x-ray intensity

Current amplifier and converter of I to V



Voltage to frequency converter and counter

Ion chamber characteristics



Efficiency of a 10-cm-long gas ionization chamber as a function of energy, for different gases at normal pressure.
The efficiency of the detector can be calculated from the active length of the chamber, the properties of the chamber gas, and the x-ray absorption cross section at the appropriate photon energy

Once the efficiency is known, the photon flux can be estimated from chamber current and the average energy required to produce an electron-ion pair

Element	Energy (eV)
Helium	41
Nitrogen	36
Air	34.4
Neon	36.3
Argon	26
Krypton	24
Xenon	22

Photon flux evaluation

$$I = Ne = I_0 T \gamma e$$

I_0 = Incoming photon flux (ph/s)

T = Ion chamber window transmission

γ = gas efficiency (electrons/ph)

L = length of the ion chamber plate

$$N \cong \frac{E}{\langle V_i \rangle}$$

N = Number of electron-ion pairs produced

E = X ray energy

$\langle V_i \rangle$ = Average energy required to produce an electron-ion pair

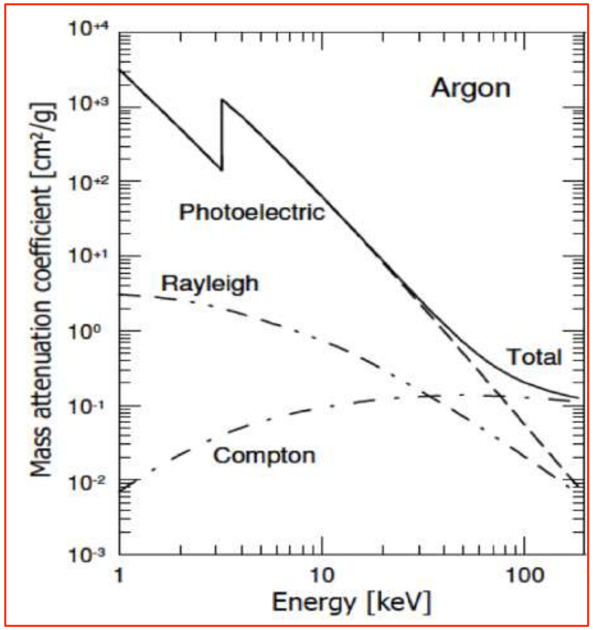
$$I_0(ph/s) = \frac{I(A)}{\gamma e(C)} \frac{\langle V_i \rangle (eV)}{E(eV)} \frac{1}{1 - e^{-\mu L(cm)}}$$

$$\mu(cm^{-1}) = \left[\frac{\mu}{\rho}(E)\right] \rho$$

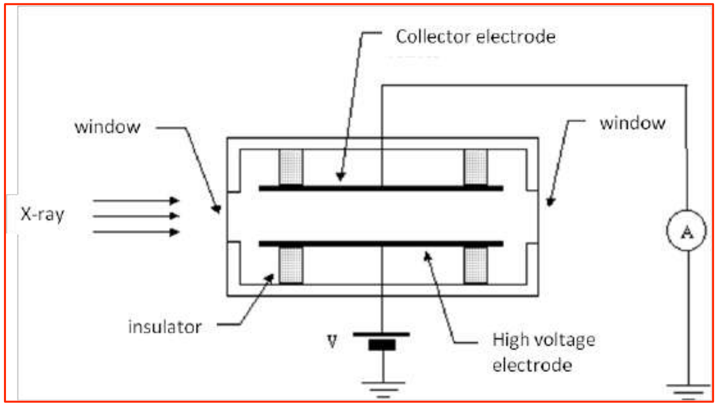
$\left[\frac{\mu}{\rho}\right]$ = gas mass attenuation coefficient

ρ = gas density function of pressure (γ)

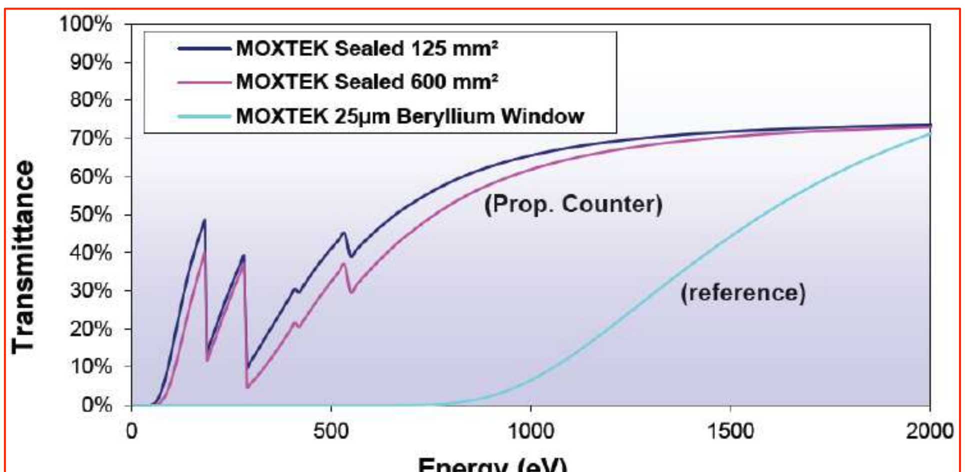
γ = I_0 10%; I_1 90%



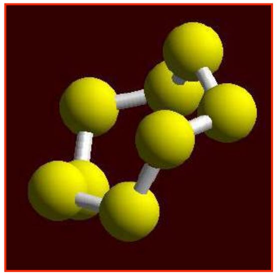
X-ray ion chambers ad windows



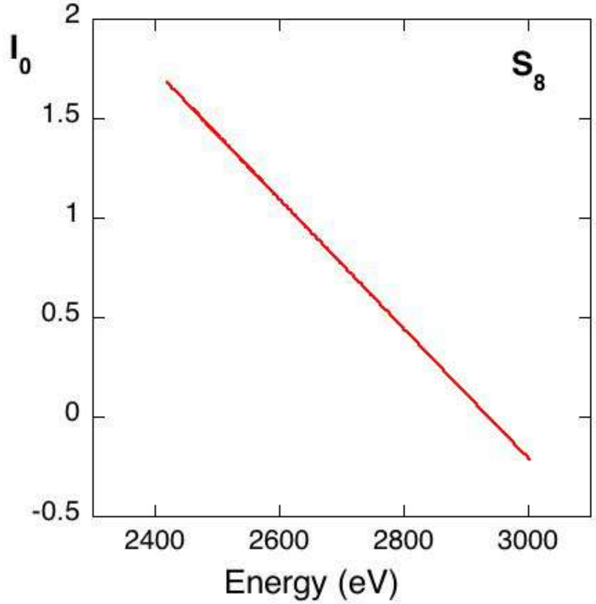
Unmounted and mounted MOXTEK ultrathin windows



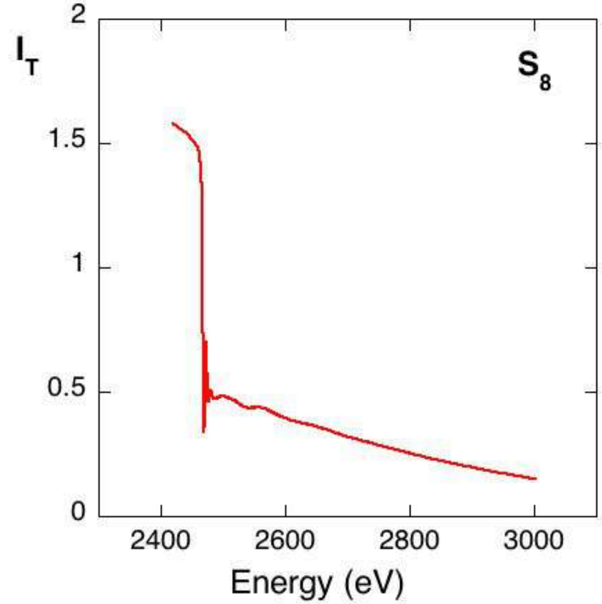
XAFS S_8



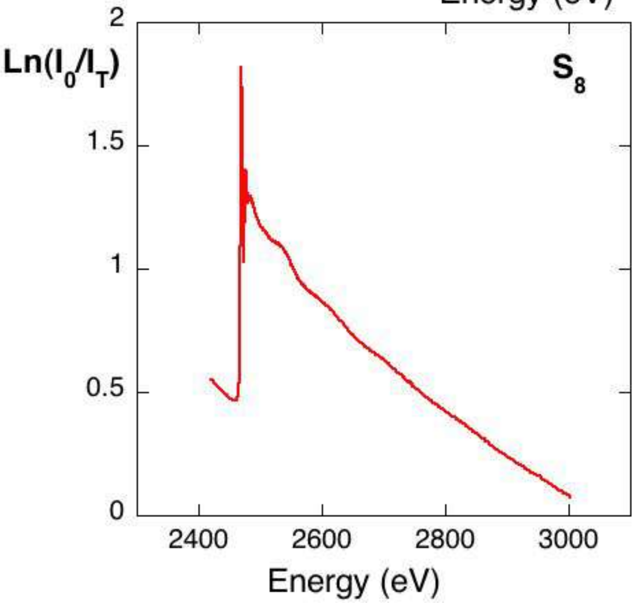
S_8



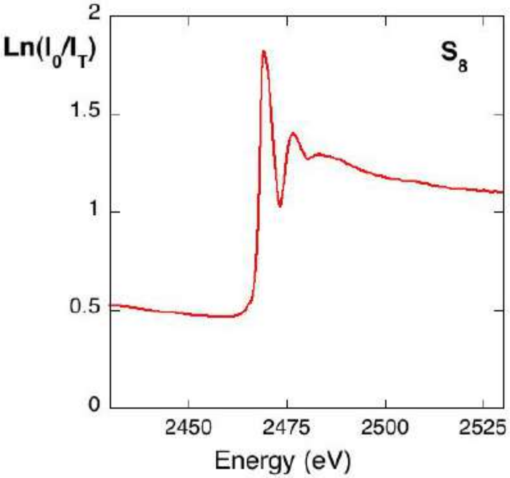
I0
S8
2
1.5
1
0.5
0
-0.5
2400
2600
2800
3000
Energy (eV)



IT
S8
2
1.5
1
0.5
0
2400
2600
2800
3000
Energy (eV)



Ln(I0/IT)
S8
2
1.5
1
0.5
0
2400
2600
2800
3000
Energy (eV)



Ln(I0/IT)
S8
2
1.5
1
0.5
0
2450
2475
2500
2525
Energy (eV)

Thank you for your attention

Supplementary material

Reminder

- *Speed of light* — $c = 2.99792458 \times 10^8$ m/s
- *Electron charge* — $e = 1.6021 \times 10^{-19}$ Coulombs
- *Electron volts* — $1\ eV = 1.6021 \times 10^{-19}$ Joule
- *Energy and rest mass* — $1 eV/c^2 = 1.78 \times 10^{-36}$ kg

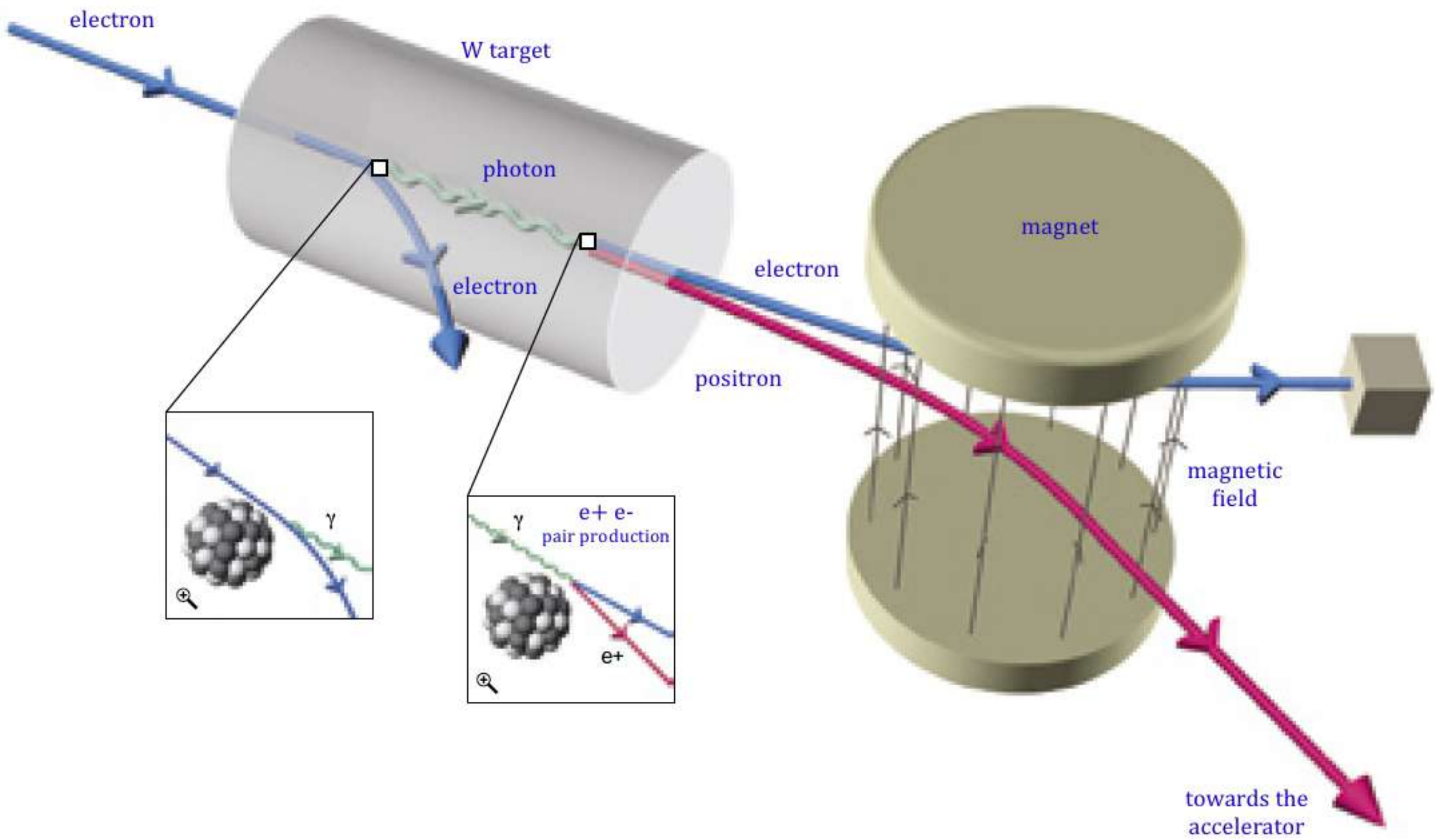
  Electron — $m_0 = 511.0\ keV/c^2 = 9.109 \times 10^{-31}$ kg

  Proton — $m_0 = 938.3\ MeV/c^2 = 1.673 \times 10^{-27}$ kg
- *Relativistic energy, E* — $E = mc^2 = m_0 \gamma c^2$
- *Lorentz factor, γ* — $\gamma = 1/[(1-v^2/c^2)^{1/2}] = 1/[(1-\beta^2)^{1/2}]$

  $\beta = v/c$
- *Relativistic momentum, p* — $p = mv = m_0 \gamma \beta c$
- *E-p relationship* — $E^2/c^2 = p^2 + m_0 c^2$

  for ultra-relativistic particles — $\beta \approx 1$, $E = pc$
- *Kinetic energy* — $T = E - m_0 c^2 = m_0 c^2 (\gamma - 1)$

Anti-matter positron production



M. Calvetti, *Antiparticelle accelerate*, ***Asimmetrie*** 7, 16-21 (***2008***)