Synchrotron techniques for materials characterization

X-ray generation, interaction and detection

Berit Zeller-Plumhoff

Data-Driven Analysis and Design of Materials

Universität Rostock

Open position(s) for student assistants / theses projects

1. **Design and implementation of online lecture „Synchrotron techniques for materials characterization“**

2. Modelling of chronic inflammation in skin pathologies

3. Modelling of angiogenesis near biodegradable implants

4. (Data-driven) Modelling of biofouling and anti-fouling strategies

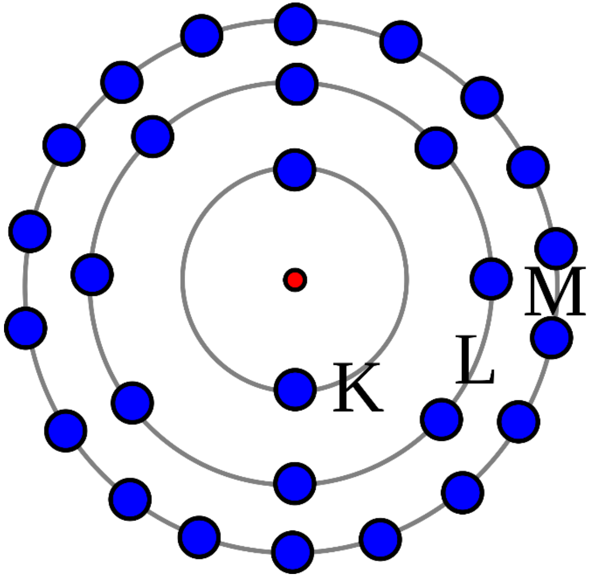
Learning goals

At the end of the lecture you will

- Be familiar with the main components of a synchrotron and their function
- Understand in which manner X-rays can interact with matter
- Understand the requirements for X-ray detection

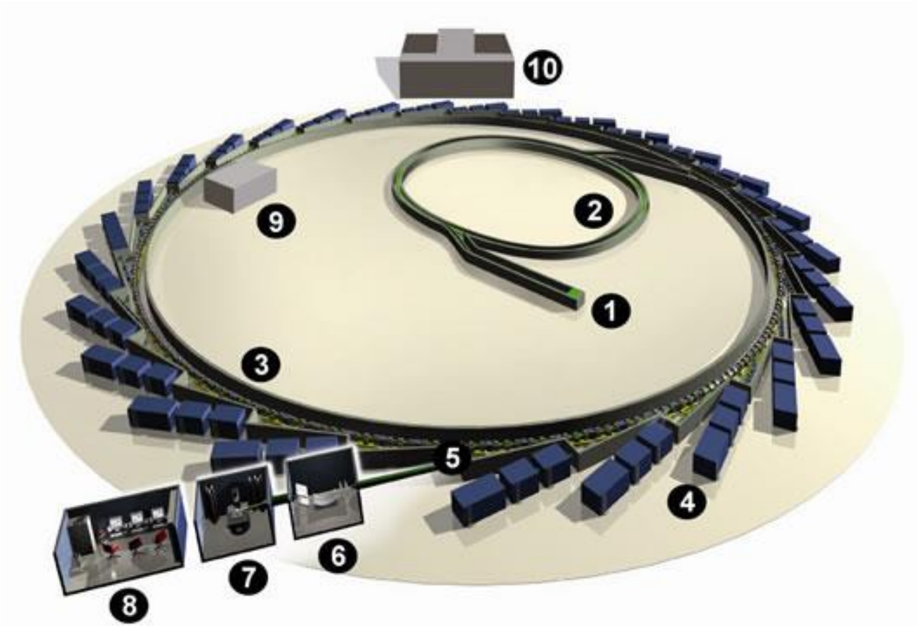
Atoms

Bohr model (1921)



https://en.wikipedia.org/wiki/Bohr_model

What is a synchrotron



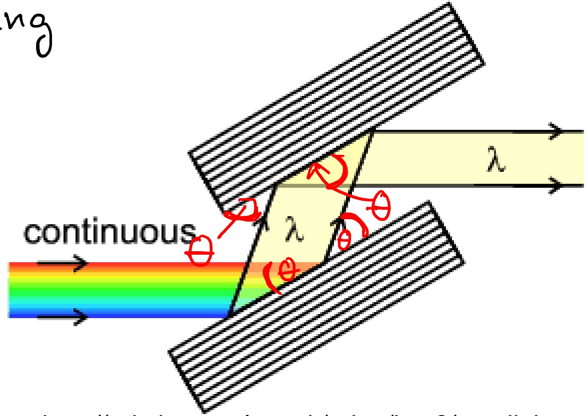
https://www.diamond.ac.uk/Science/Machine/Components.html

Monochromator

- perfect crystal
- selection of angle determine the outgoing wavelength

→ Bragg's law: $\underbrace{m}_{\text{integer multiple}} \underset{\text{wavelength}}{\tilde{\lambda}} = 2\underbrace{d}_{\text{lattice spacing}} \sin \underbrace{\theta}_{\text{refraction angle}}$

- relative wavelength band $\xi = \frac{\Delta\lambda}{\lambda}$ (not infinitely sharp response)
- silicon, diamond, germanium

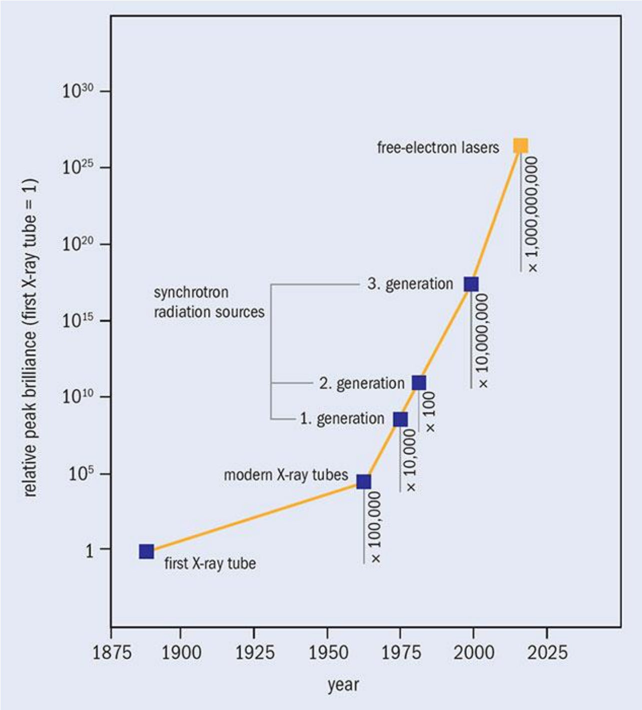


http://pd.chem.ucl.ac.uk/pdnn/inst2/condit.htm

Brilliance

$$\text{brilliance} = \frac{\text{Photons / second}}{\underbrace{(\text{mrad})^2}_{\substack{\text{angular}\\ \text{divergence}}} \underbrace{(\text{mm}^2)}_{\substack{\text{source}\\ \text{area}}} \underbrace{(0.1\%\ \text{BW})}_{\substack{\text{band with}\\ \text{(spectral distribution)}}}}$$

Brilliance



J.-A. Nielsen, Elements of Modern X-ray Physics

Virtual tour through PETRA III

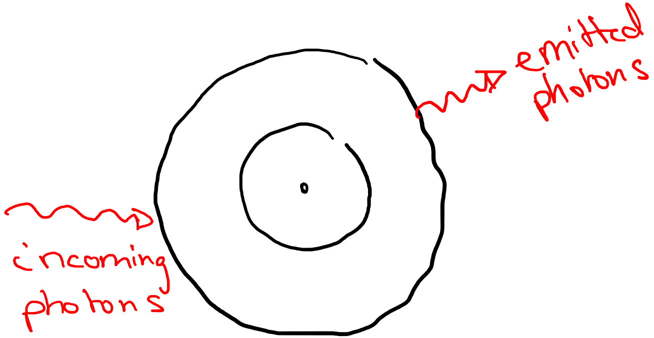
https://vtour.desy.de/desytour/index_de.html

X-ray interaction with matter

- energy dependent
- 4 main interactions
  - coherent scattering
  - photoelectric effect
  - Compton scattering
  - pair production

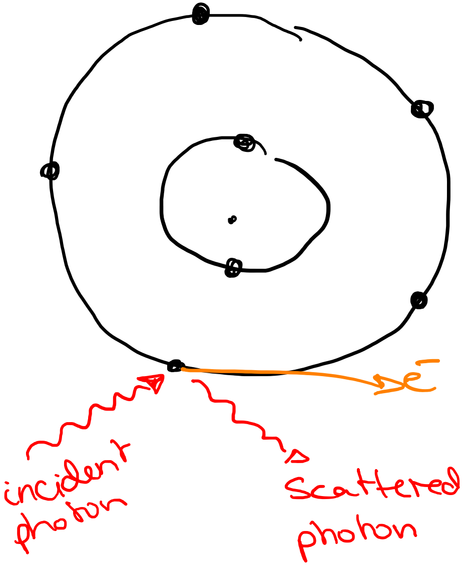
!

Coherent scattering



- Photon interacts with electron cloud
  - → movement then relaxation
  - → re-emission of photons of same frequency
- scattering mainly forward
- main interaction in X-ray crystallography (X-ray diffraction, small angle X-ray scattering)
- cross-section : σ_{coh} → measure of efficiency of scattering

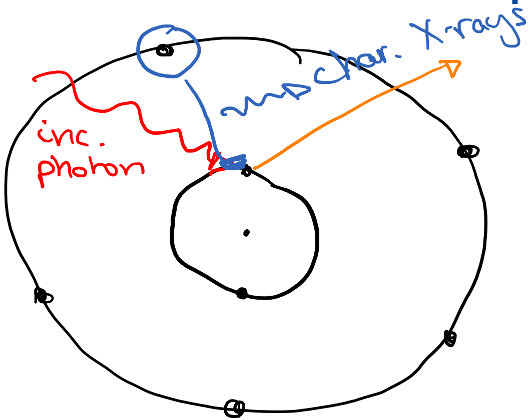
Compton scattering



incoherent scattering σ_{incoh}

- interaction of photon with outer shell electron or free electron
- scattering of photon
  => loss of energy => different wavelength
- main mode of contrast mode for clinical CT

Photoelectric absorption



- photon absorption
- ejection of inner shell electron
  - → relaxation of outer shell electron
  - → characteristic X-rays
- $\sigma_{pe} \propto \frac{Z^3}{E^3}$ => dominant for high-Z materials and energies up to ~300 keV
- main contrast mode for imaging in µCT & nano CT

Mass attenuation coefficient

total cross-section

$$\sigma_{tot} = \sigma_{incoh} + \sigma_{coh} + \sigma_{pe}$$

mass attenuation coefficient

$$\frac{\mu}{\rho} = \frac{\sigma_{tot}}{uA}$$

μ - linear attenuation coefficient

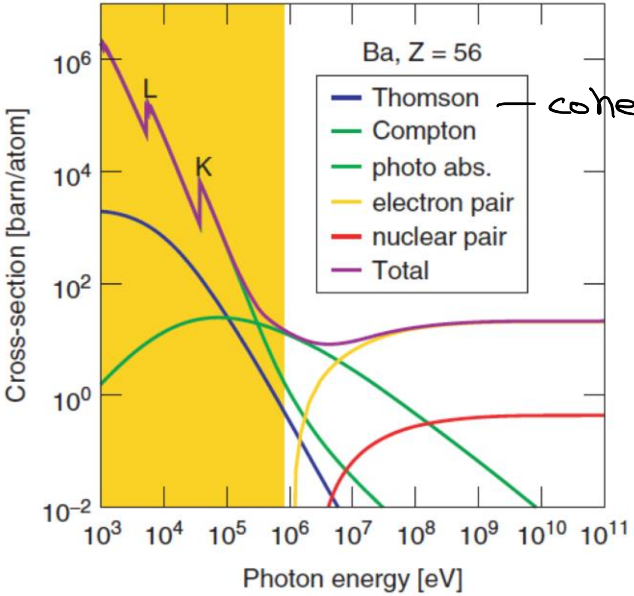
ρ - density of material

u - $1.66 \cdot 10^{-24}$ g atomic mass unit

A - relativ atomic mass of elements

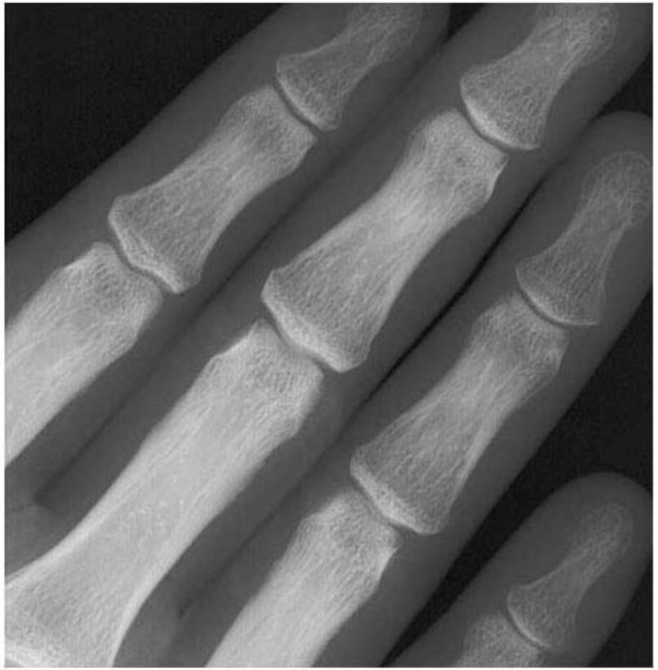
Interaction of X-rays with matter

Cross Section of Ba



coherent scattering

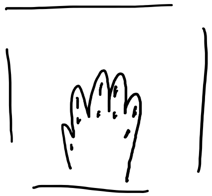
X-ray detection

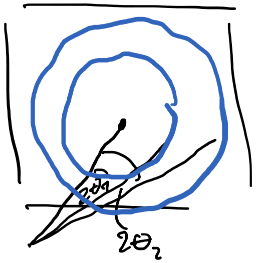


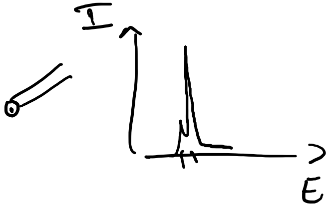
http://sharp-world.com/corporate/info/rd/tj3/pdf/6.pdf

Application-dependency of detector

- imaging → determine intensity distribution
- scattering → determine intensity as function of scattering angle
- spectroscopy → determine intensity and energy of X-ray



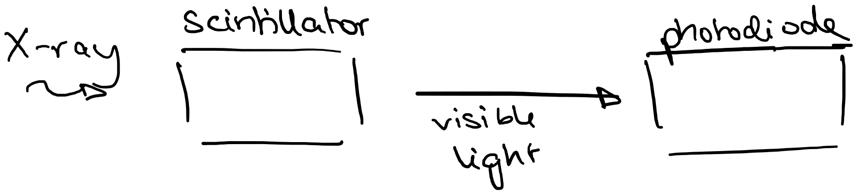


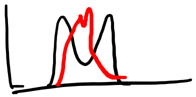


Principle of X-ray detection

1. X-ray light is quantized (photon)
2. Transfer energy from photon to detector
3. Photon is neither fully absorbed nor not at all
4. Transfer of energy into electrical signal and then number

Requirements of scintillation





- absorption of energy and re-emission
- requirements:
  - high yield
  - small time constant
  - good linearity
  - transparent to scintillation light
  - good mechanical properties
  - temperature stable
    → most of X-ray energy lost as heat

Principle and efficiency of scintillation

- inorganic crystal scintillators (CsI, NaI, $LaCl_3$)
- electronic band structure
- electron from valence band is excited onto conduction band by X-ray
- migrates through material to impurity centre
  → de-excitation → emission of visible light

efficiency of scintillation η

$$\eta = \frac{E_{vis}\, N_{ph}}{E_{X\text{-}ray}} \quad ?$$

E_{vis} - energy of visible light
$E_{X\text{-}ray}$ - " —— X-ray
N_{ph} - number of vis. light photons

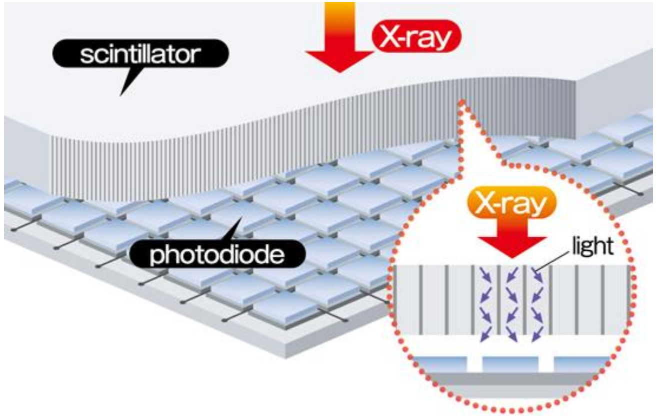
usually $\eta \approx 0.2$

Conversion into electrical signal

- photodiode (semi conductor)
- CCD, CMOS chips

Conversion into electrical signal

https://www.ugent.be/we/ugct/en/research/ctscanners



https://www.konicaminolta.com/healthcare/products/dr/dr30/index.html