DTU

22485 lectures

# X-ray physics

# Plan for lecture

- Introduction to X-rays
- X-ray sources
- X-ray 2D Imaging
- X-ray interaction with matter
- X-ray detectors
- X-ray safety and doses

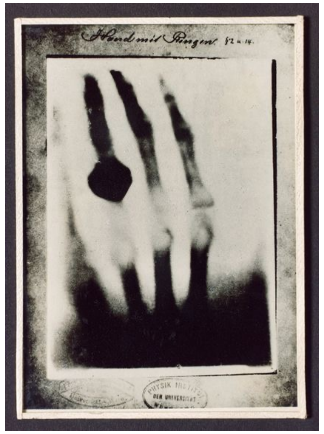
# NEutrons and X-rays for MAterials Physics

- Methods development for material science
- Instrument development
- Software development
- Material physics
- Use of Large scale facilities

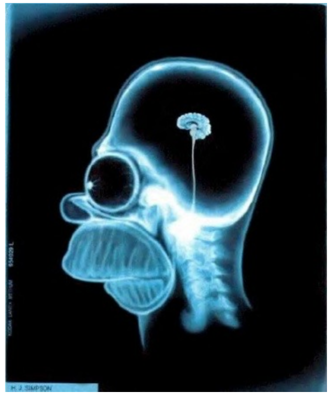
Introduction to X-rays

# X-rays and why use them

- Wilhelm Rontgen discovered X rays in 1895
- High penetration of X rays in materials makes probing of buried structures possible
- Even Superman uses x-ray vision to see through solid objects surface

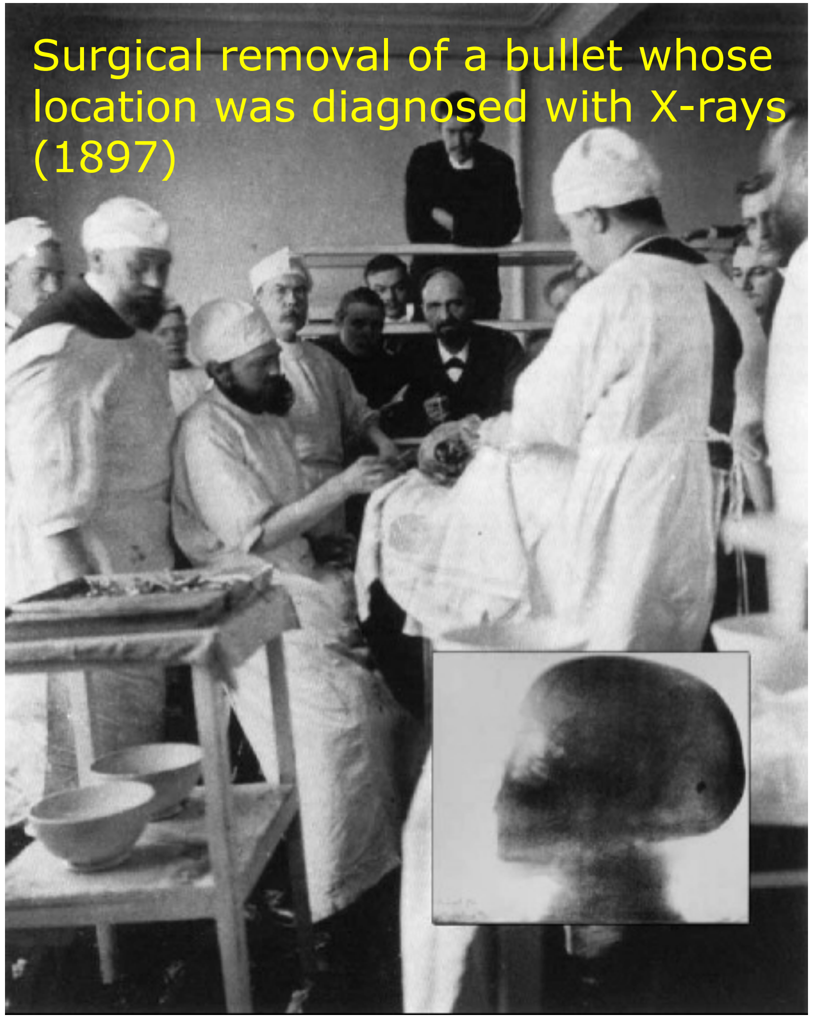
*The print of the first x-ray image (right) taken on December 22$^{nd}$ 1895. The hand belonged to Anna Bertha, the wife of German physicist Wilhelm Röntgen (left).*

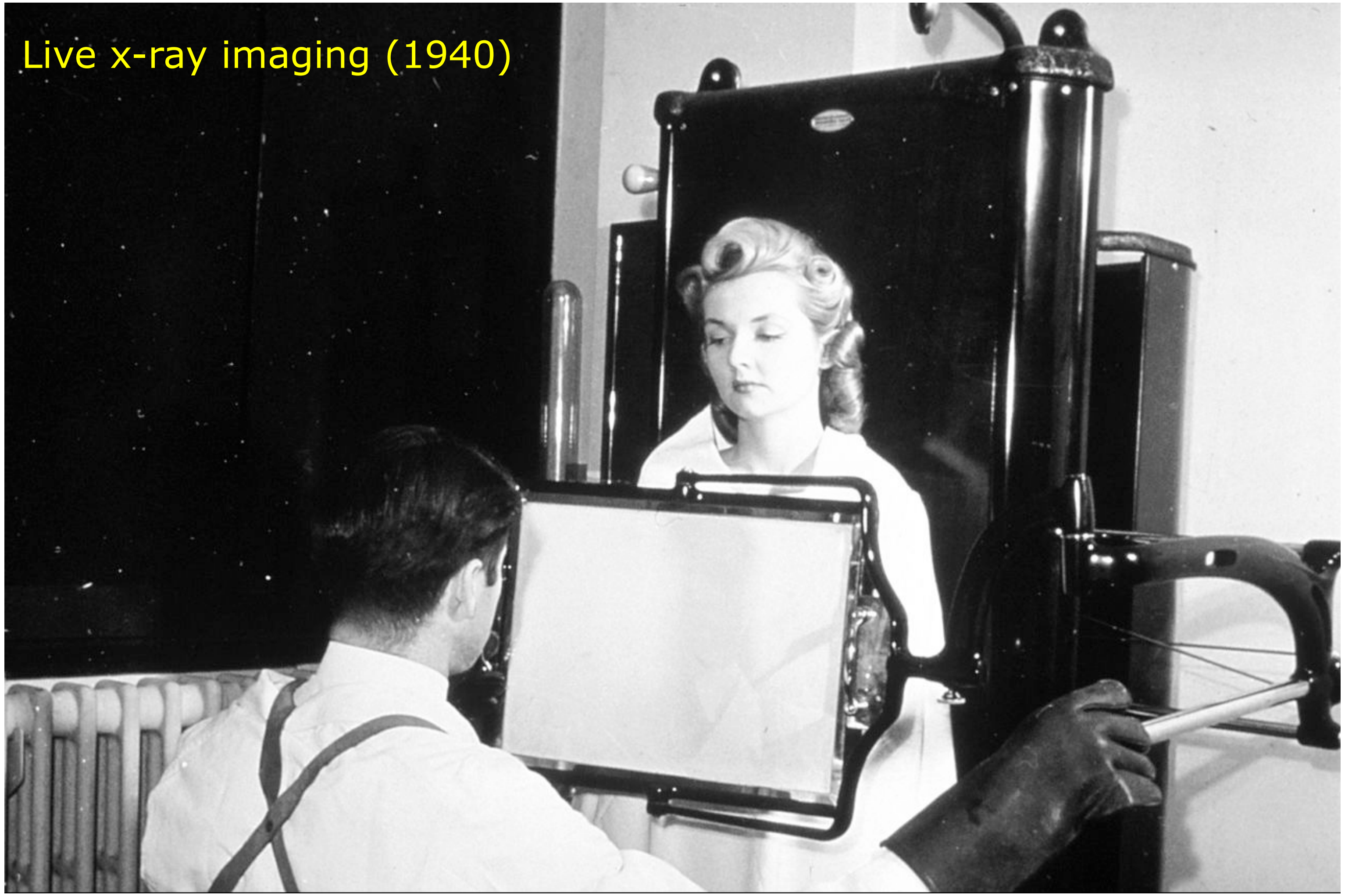



# X-rays and why use them

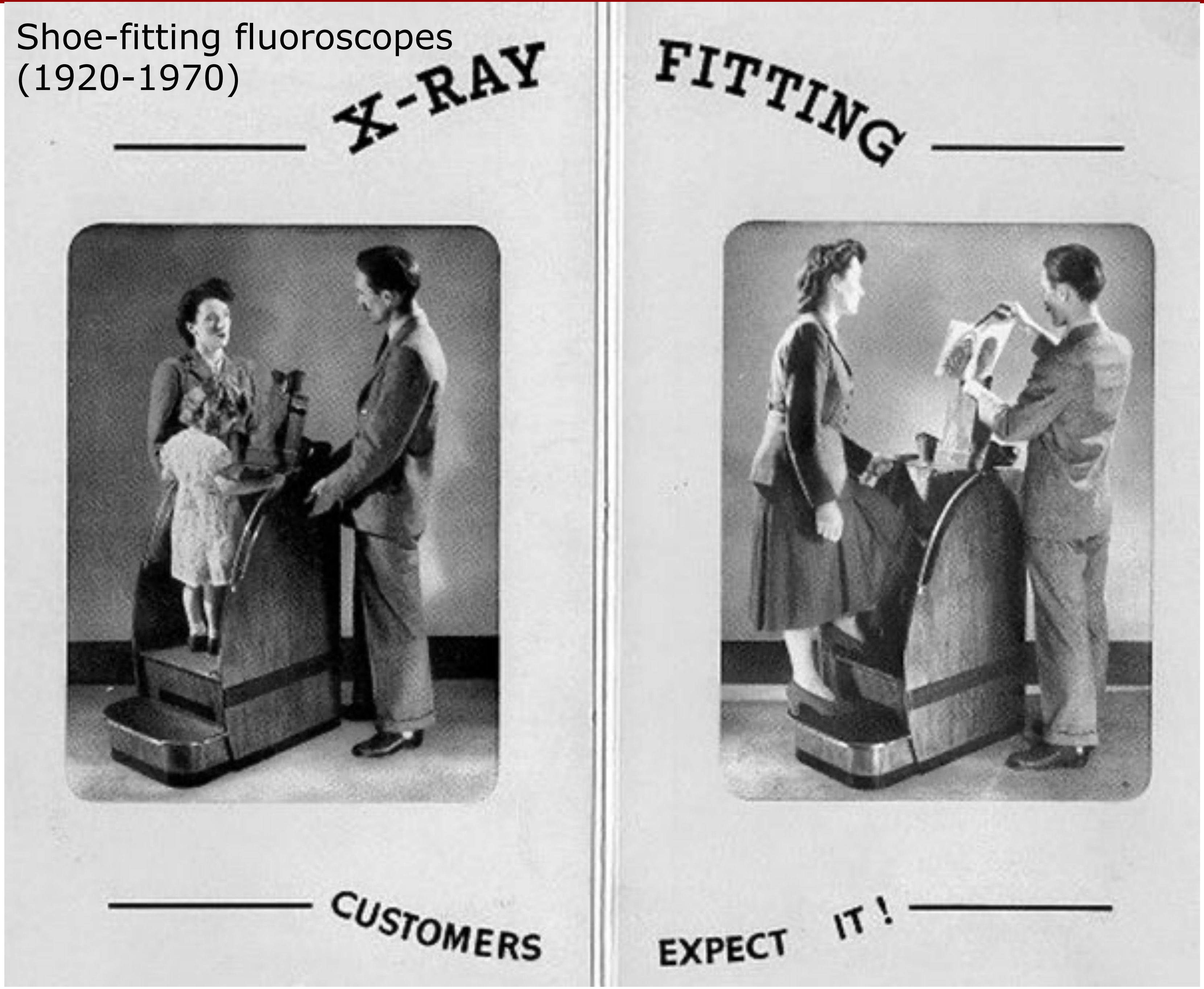
- X-rays give rapid, high resolution anatomical information(many photons, good S/N)
- Rapid introduction and simple technology

# Early medical applications



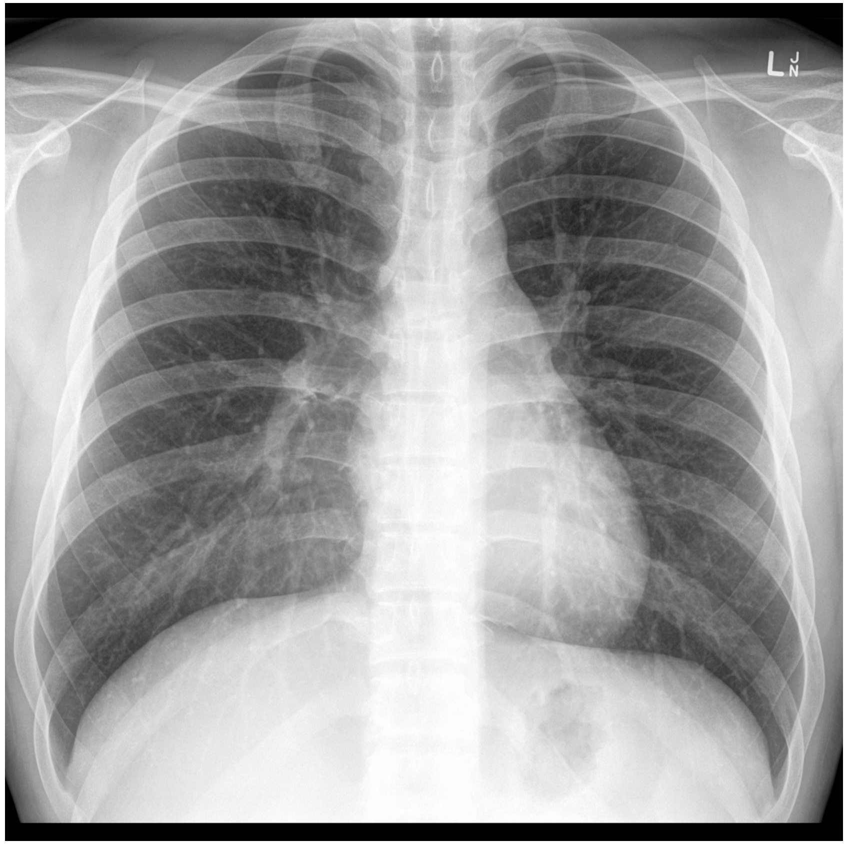



# Shoe-fitting fluoroscopes (1920-1970)



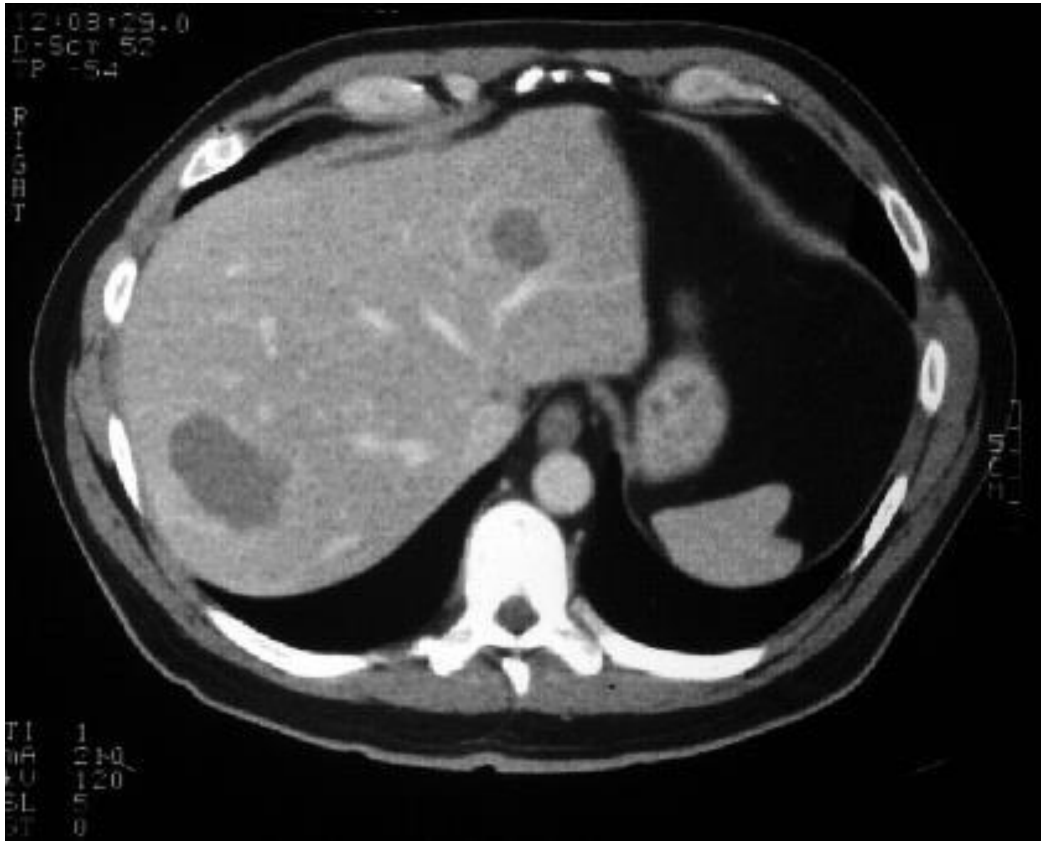
# X-ray Imaging

Planar X-ray Imaging



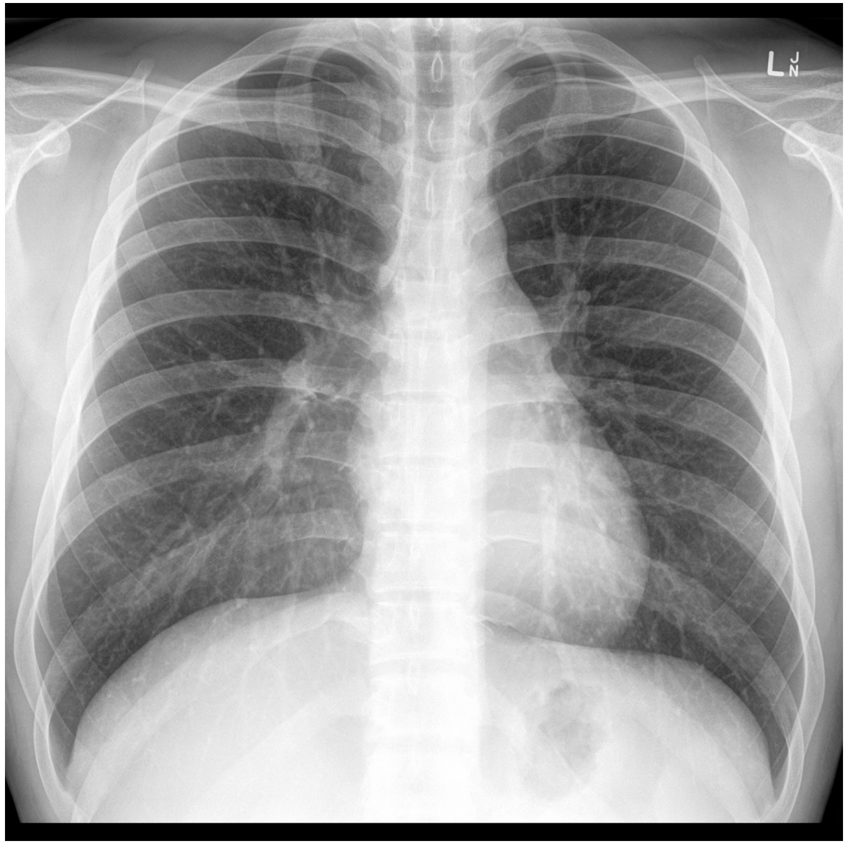
Case courtesy of Assoc Prof Frank Gaillard, Radiopaedia.org, rID: 8090

X-ray tomography (CT)



# X-ray Imaging

Planar X-ray Imaging

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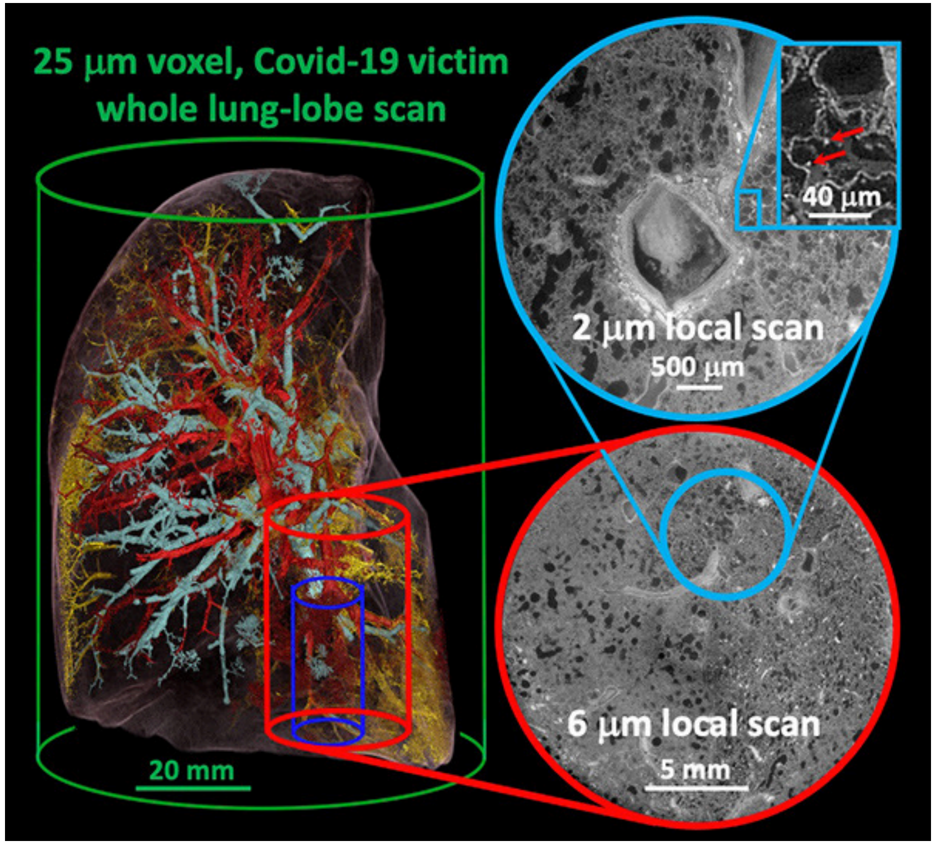
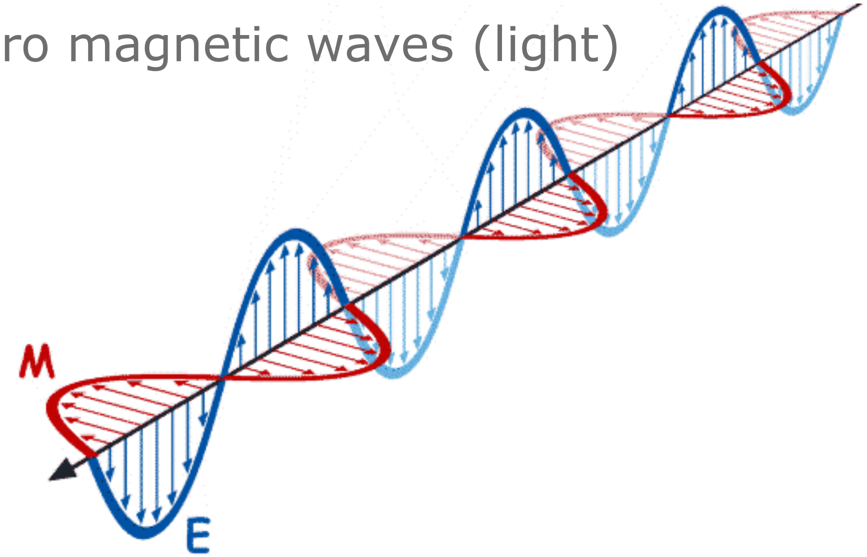
X-ray tomography (CT)




Credit: P.Tafforeau/ESRF

# X-ray properties

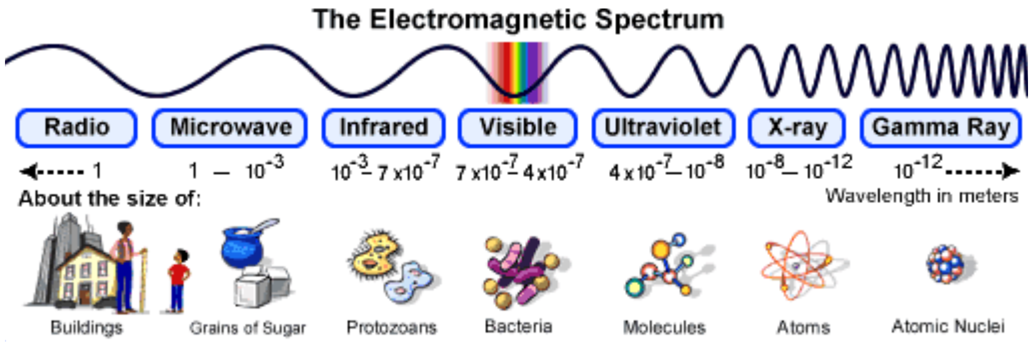
Electro magnetic waves (light)




Wavelength ~ $1^{-10}$ m (1 Å)

Interference with matter:

- **Scattering**
- **Photoabsorption**



# Wave/Particle duality

**X-rays are mass-less particles with an energy, $E = h\omega$**

where $h$ is planck constant, and $\omega$ is its frequency

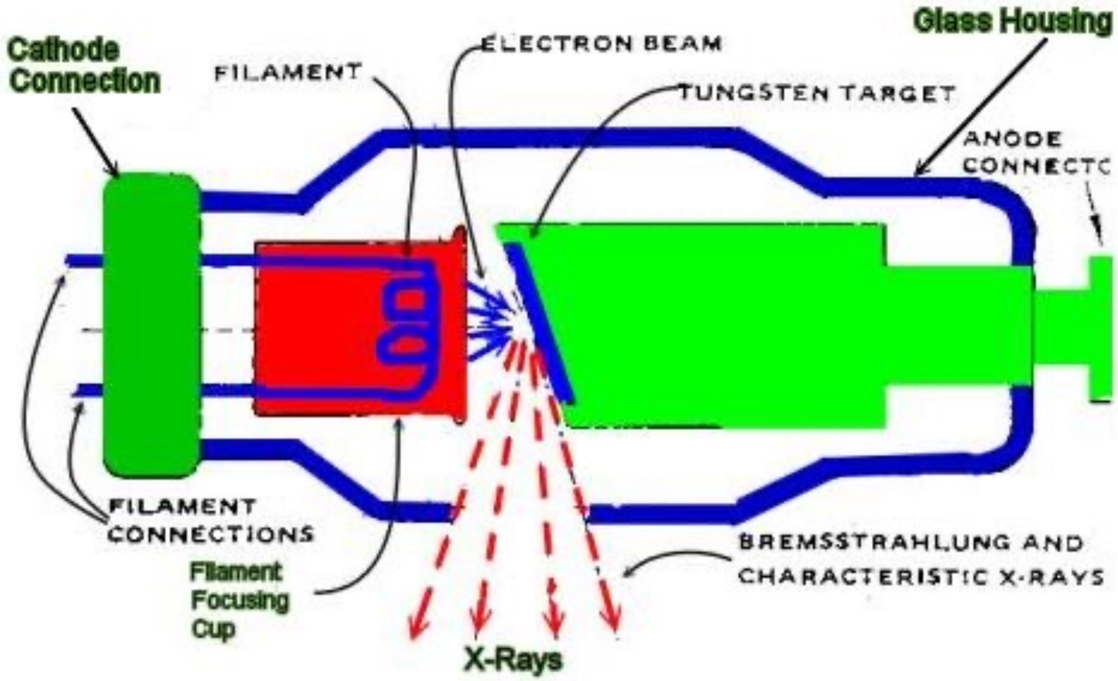
**X-rays are electromagnetic waves with amplitude and wavelength, $\lambda$ with an energy, $E = hc/\lambda$**

where $c$ is the speed of light

# X-rays sources

# X-ray Generation

- Electrons are emitted by a cathode, strike an anode containing a target material.
- Electrons excite the atoms in the target material, which release energy in the X-ray spectrum



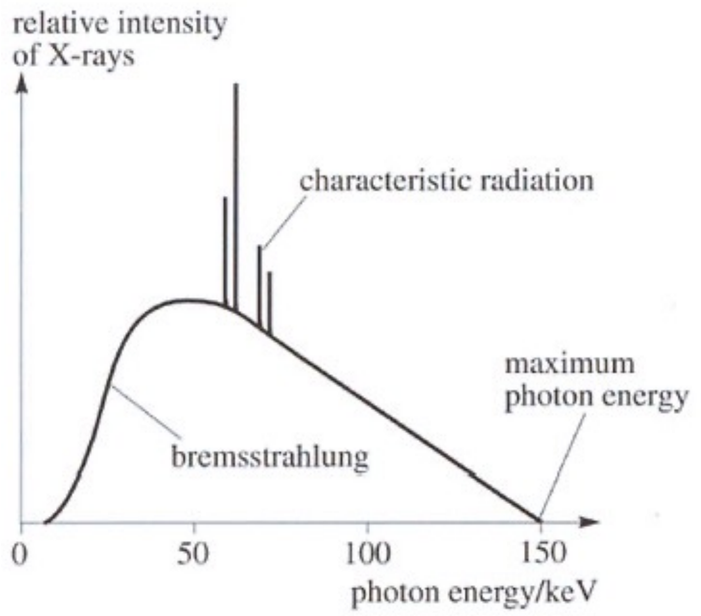
# Target Materials & X-ray Spectra

- Different target materials produce different characteristic emission lines, as well as different broad-band emission spectra all the way up to the accelerating voltage (*bremsstrahlung*)
- Common target materials:
  - **Tungsten (W)**, Copper (Cu), Vanadium (V), Chromium (Cr), Molybdenum(Mo)

| Element | $K\alpha_1$ | $K\alpha_2$ | $K\beta_1$ | $L\alpha_1$ | $L\alpha_2$ | $L\beta_1$ | $L\beta_2$ | $L\gamma_1$ | $M\alpha_1$ |
|---|---|---|---|---|---|---|---|---|---|
| 63 Eu | 41,542.2 | 40,901.9 | 47,037.9 | 5,845.7 | 5,816.6 | 6,456.4 | 6,843.2 | 7,480.3 | 1,131 |
| 64 Gd | 42,996.2 | 42,308.9 | 48,697 | 6,057.2 | 6,025.0 | 6,713.2 | 7,102.8 | 7,785.8 | 1,185 |
| 65 Tb | 44,481.6 | 43,744.1 | 50,382 | 6,272.8 | 6,238.0 | 6,978 | 7,366.7 | 8,102 | 1,240 |
| 66 Dy | 45,998.4 | 45,207.8 | 52,119 | 6,495.2 | 6,457.7 | 7,247.7 | 7,635.7 | 8,418.8 | 1,293 |
| 67 Ho | 47,546.7 | 46,699.7 | 53,877 | 6,719.8 | 6,679.5 | 7,525.3 | 7,911 | 8,747 | 1,348 |
| 68 Er | 49,127.7 | 48,221.1 | 55,681 | 6,948.7 | 6,905.0 | 7,810.9 | 8,189.0 | 9,089 | 1,406 |
| 69 Tm | 50,741.6 | 49,772.6 | 57,517 | 7,179.9 | 7,133.1 | 8,101 | 8,468 | 9,426 | 1,462 |
| 70 Yb | 52,388.9 | 51,354.0 | 59,370 | 7,415.6 | 7,367.3 | 8,401.8 | 8,758.8 | 9,780.1 | 1,521.4 |
| 71 Lu | 54,069.8 | 52,965.0 | 61,283 | 7,655.5 | 7,604.9 | 8,709.0 | 9,048.9 | 10,143.4 | 1,581.3 |
| 72 Hf | 55,790.2 | 54,611.4 | 63,234 | 7,899.0 | 7,844.6 | 9,022.7 | 9,347.3 | 10,515.8 | 1,644.6 |
| 73 Ta | 57,532 | 56,277 | 65,223 | 8,146.1 | 8,087.9 | 9,343.1 | 9,651.8 | 10,895.2 | 1,710 |
| 74 W | 59,318.24 | 57,981.7 | 67,244.3 | 8,397.6 | 8,335.2 | 9,672.35 | 9,961.5 | 11,285.9 | 1,775.4 |
| 75 Re | 61,140.3 | 59,717.9 | 69,310 | 8,652.5 | 8,586.2 | 10,010.0 | 10,275.2 | 11,685.4 | 1,842.5 |
| 76 Os | 63,000.5 | 61,486.7 | 71,413 | 8,911.7 | 8,841.0 | 10,355.3 | 10,598.5 | 12,095.3 | 1,910.2 |
| 77 Ir | 64,895.6 | 63,286.7 | 73,560.8 | 9,175.1 | 9,099.5 | 10,708.3 | 10,920.3 | 12,512.6 | 1,979.9 |
| 78 Pt | 66,832 | 65,112 | 75,748 | 9,442.3 | 9,361.8 | 11,070.7 | 11,250.5 | 12,942.0 | 2,050.5 |
| 79 Au | 68,803.7 | 66,989.5 | 77,984 | 9,713.3 | 9,628.0 | 11,442.3 | 11,584.7 | 13,381.7 | 2,122.9 |
| 80 Hg | 70,819 | 68,895 | 80,253 | 9,988.8 | 9,897.6 | 11,822.6 | 11,924.1 | 13,830.1 | 2,195.3 |
| 81 Tl | 72,871.5 | 70,831.9 | 82,576 | 10,268.5 | 10,172.8 | 12,213.3 | 12,271.5 | 14,291.5 | 2,270.6 |

X-ray emission lines for various elements

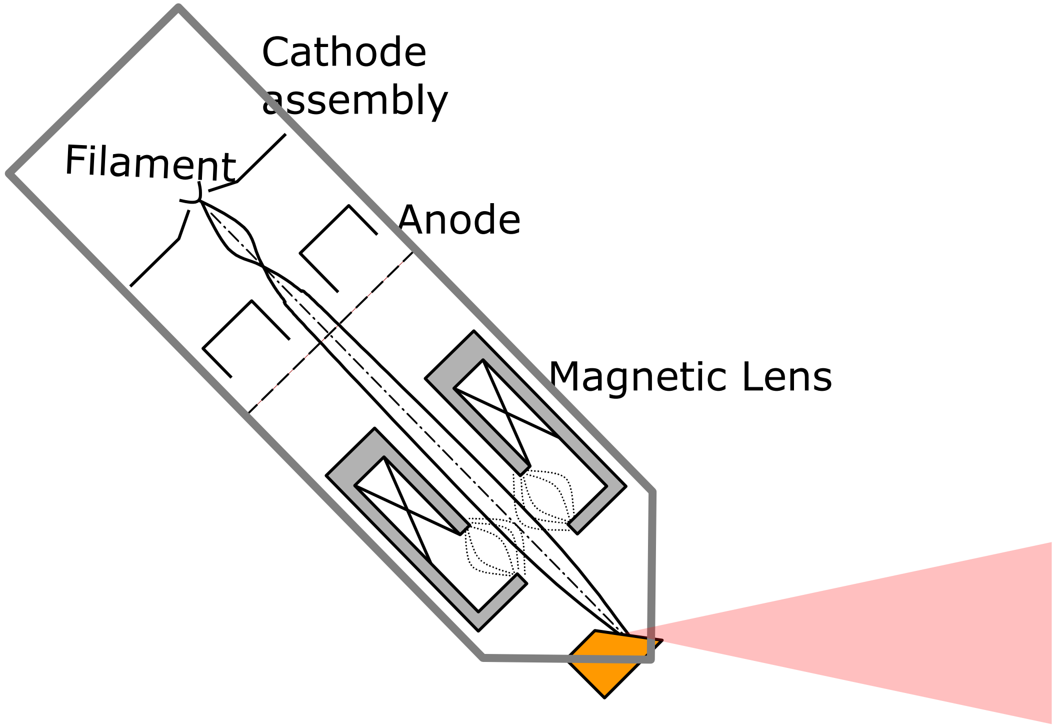
Source: X-ray Data Booklet (xdb.lbl.gov)




X-ray emission from a W laboratory X-ray source

Source: labspace.open.ac.uk

# Reflecting source

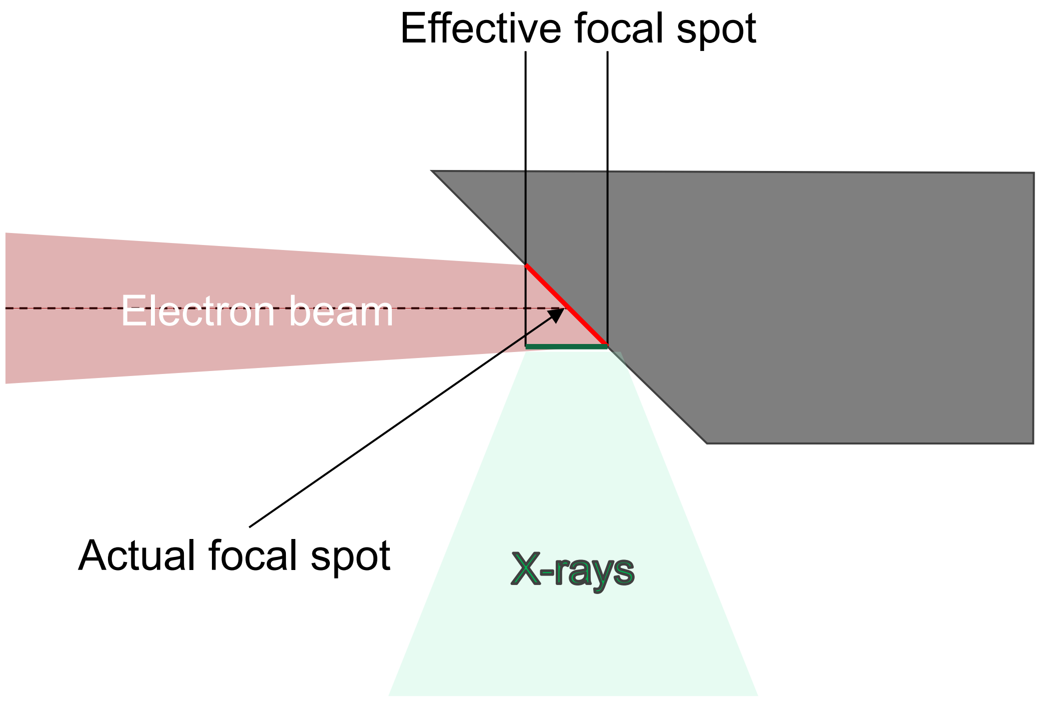


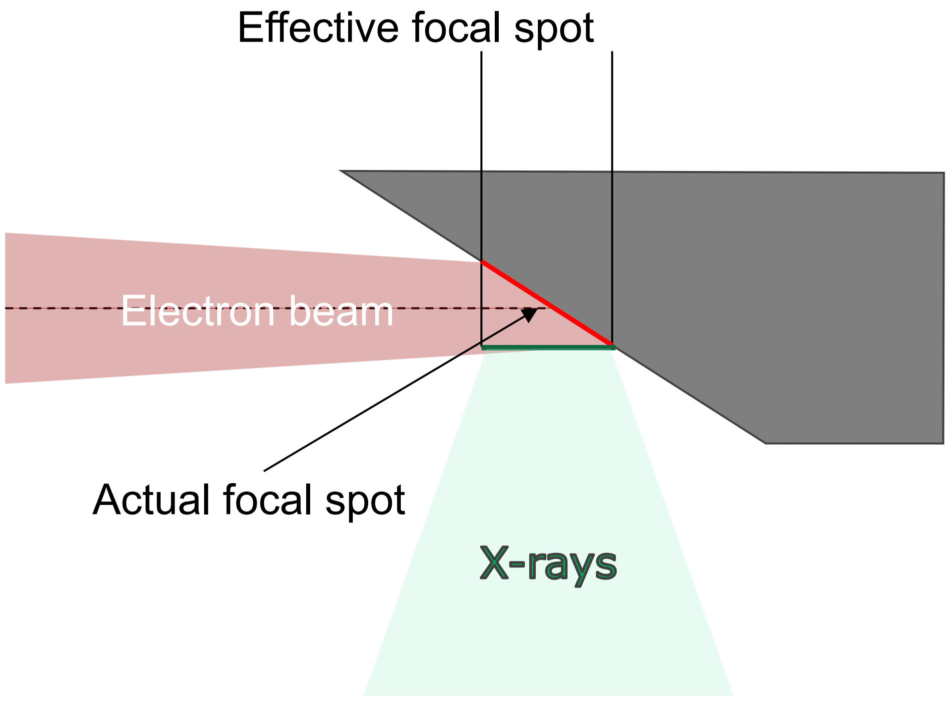


Multi-metal target: W, Ag, Mo, Cu

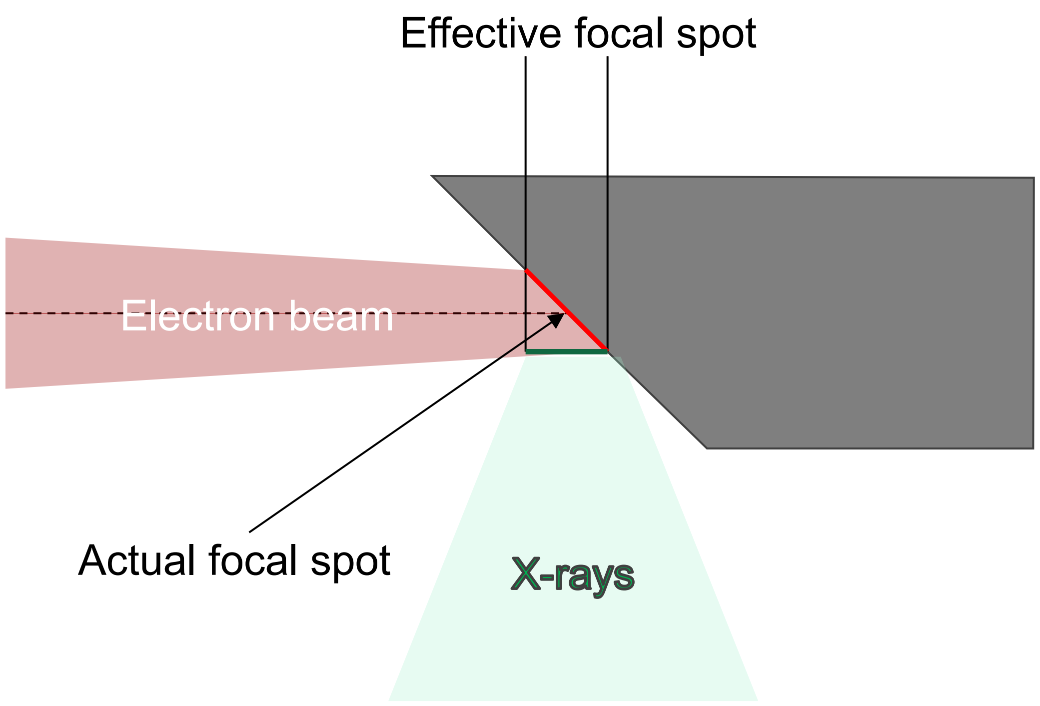
Curtesy: Nikon Metrology

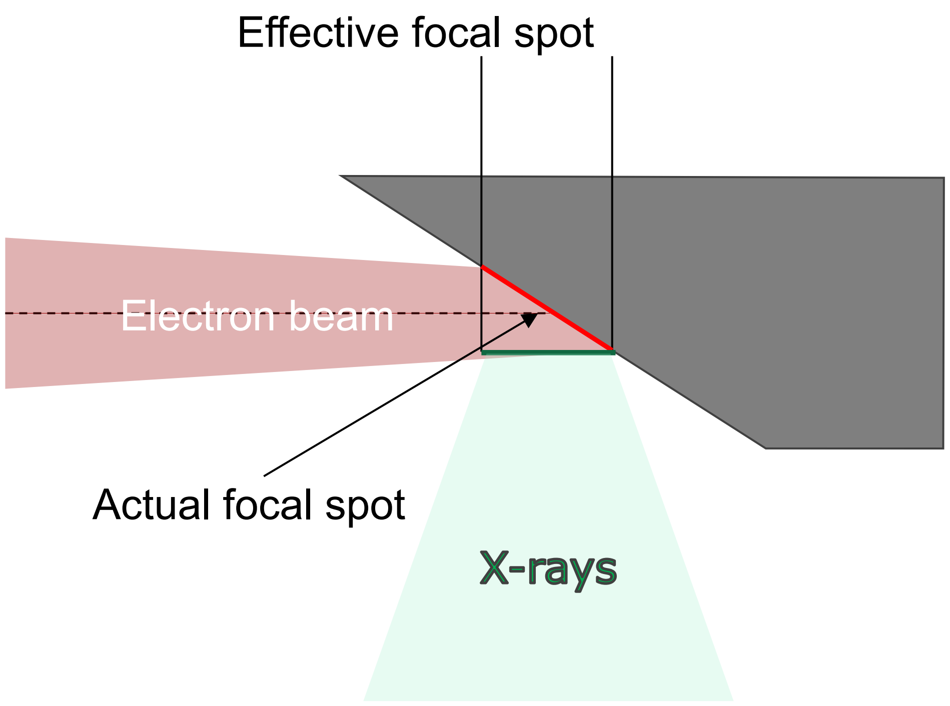
# Source focal spot



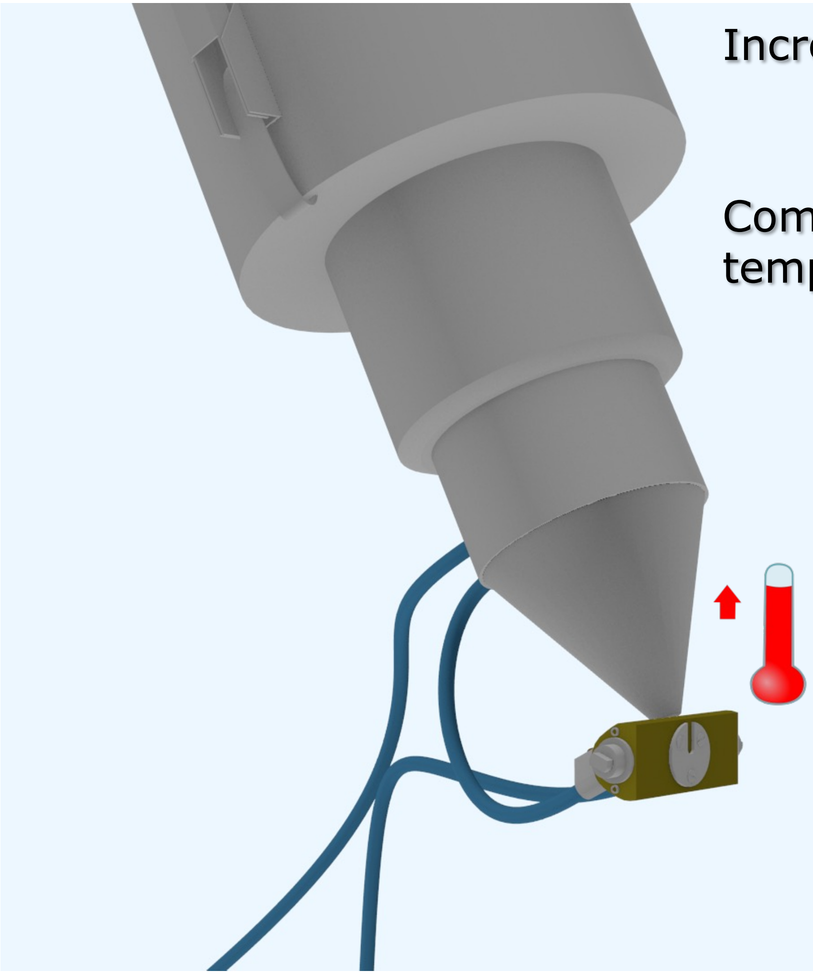



# How can you make the effective focal spot smaller?



# Standard reflection target



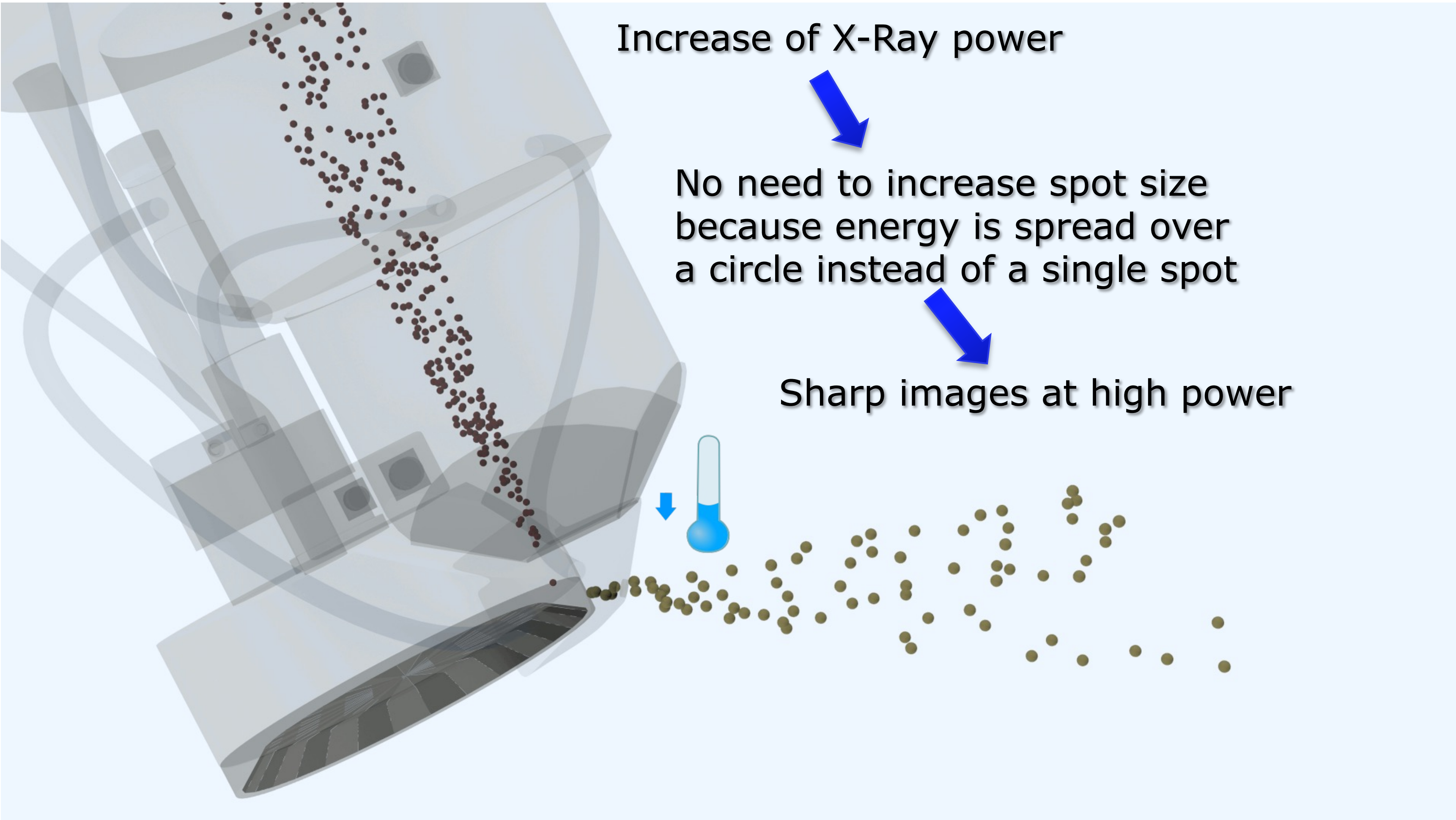
Increase of X-Ray power

Compensate increase of target temperature by increasing spot size

Decreased image resolution

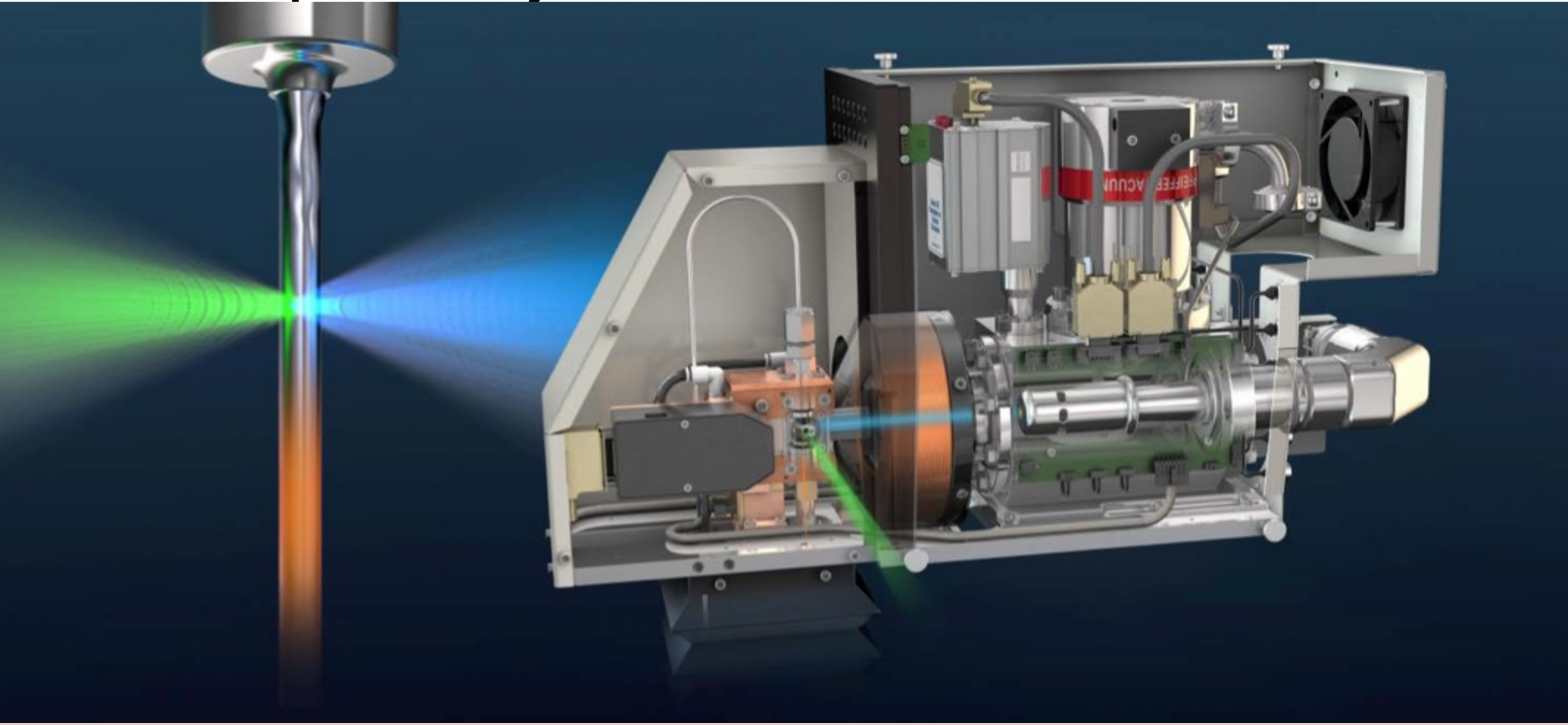
Curtesy: Nikon Metrology

# Rotating target



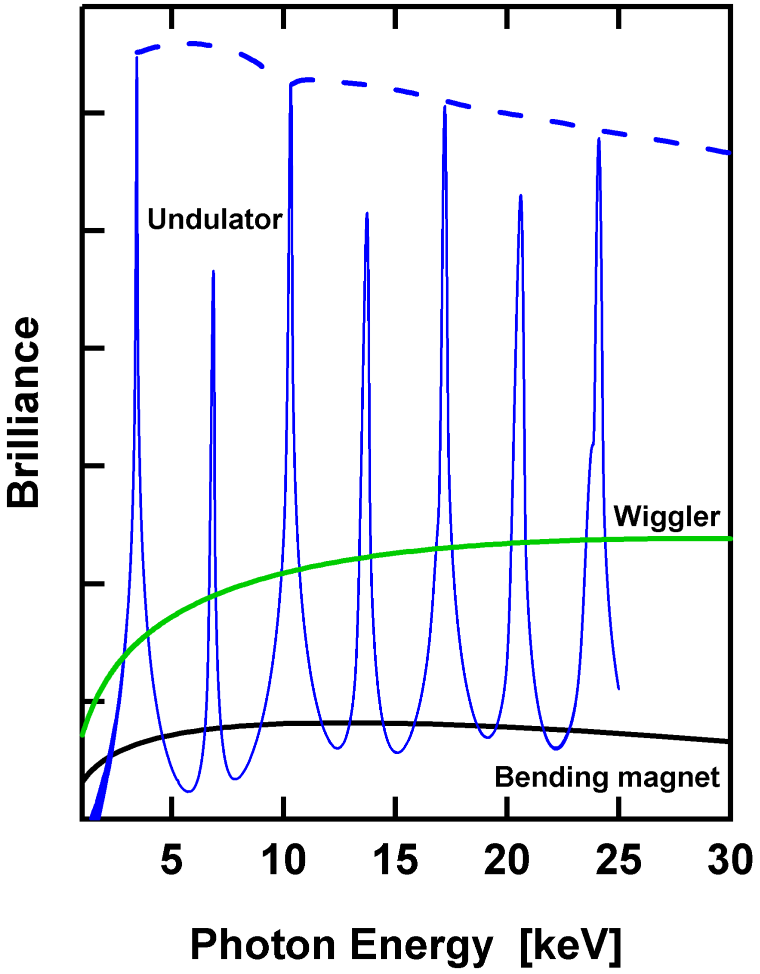

Curtesy: Nikon Metrology

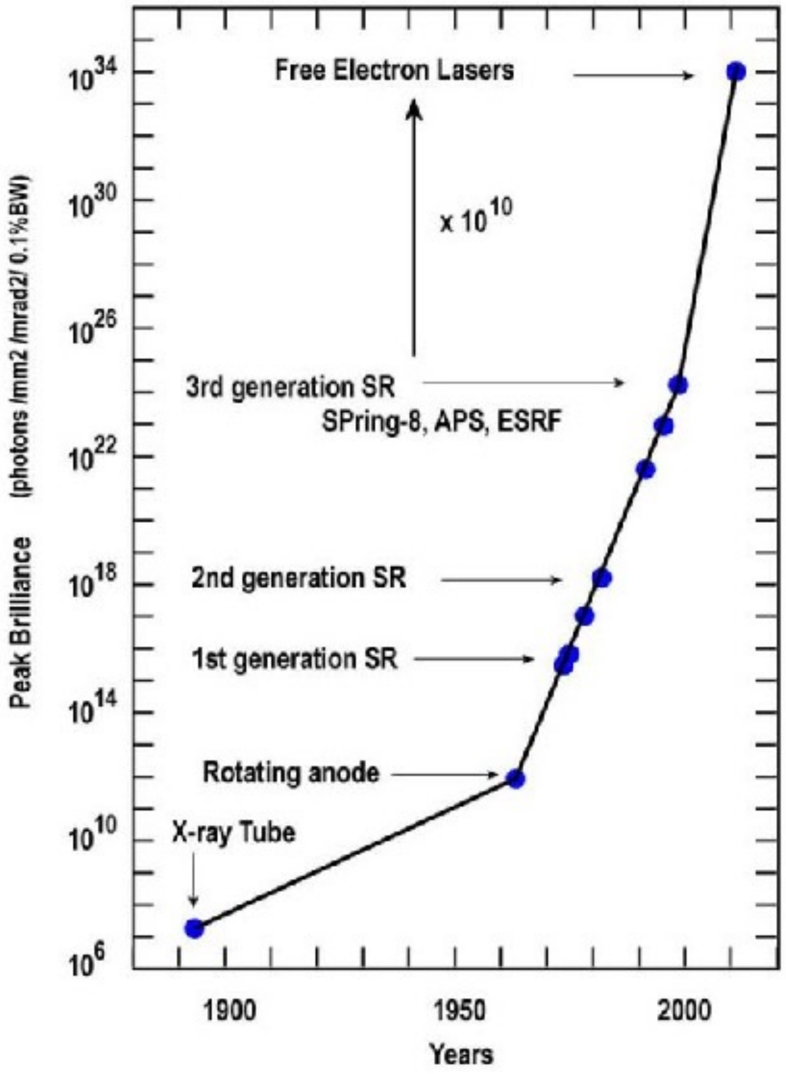
# Liquid metal jet



# Synchrotrons

# How to compare X-ray sources ?




From: http://photon-science.desy.de/research/students__teaching/primers/synchrotron_radiation/index_eng.html

Figure by: Shintake, T. (2007). Review of the worldwide SASE FEL development. Proceedings of the IEEE Particle Accelerator Conference. 89 - 93. 10.1109/PAC.2007.4440331.

# Spatial resolution and time resolution

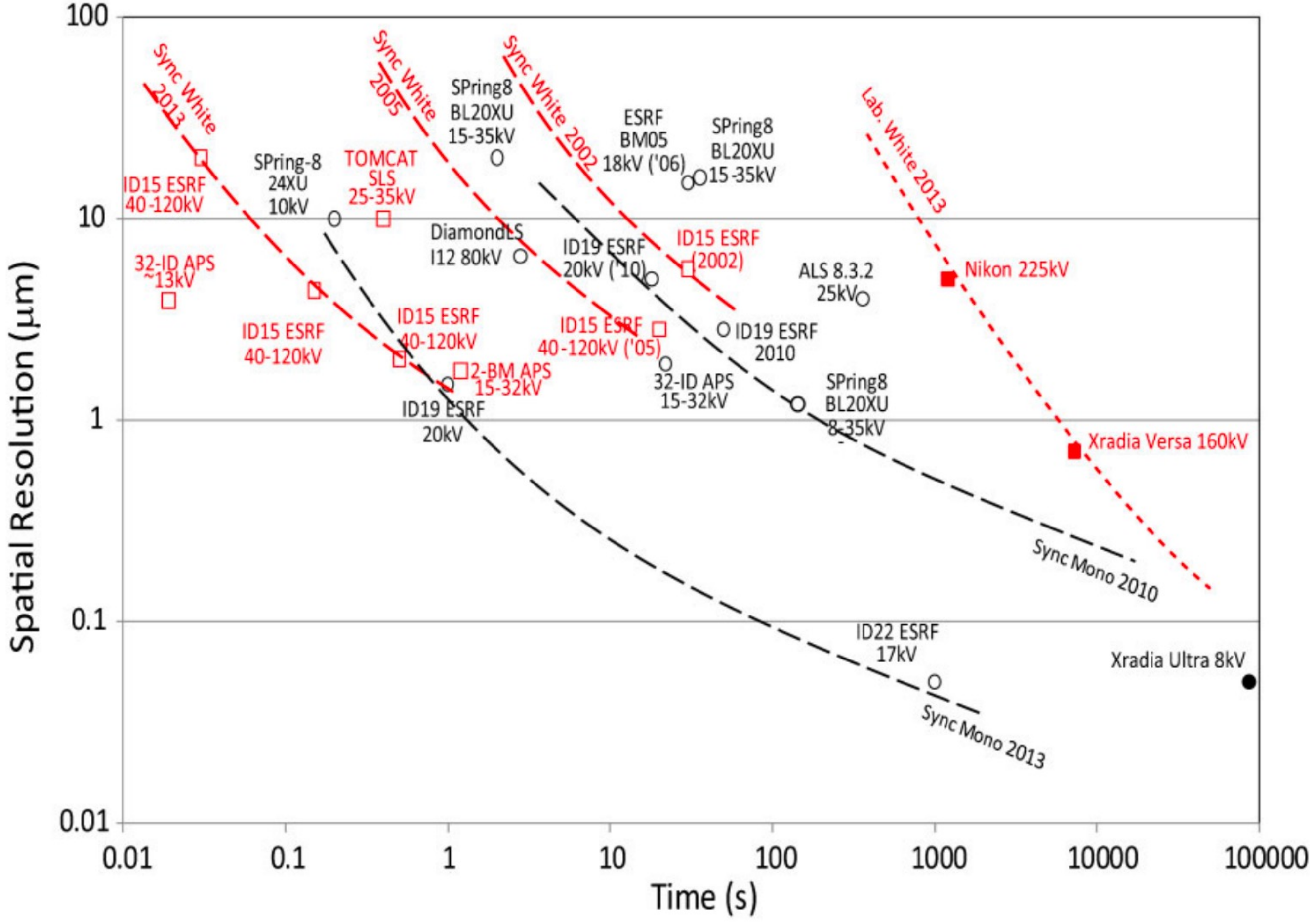


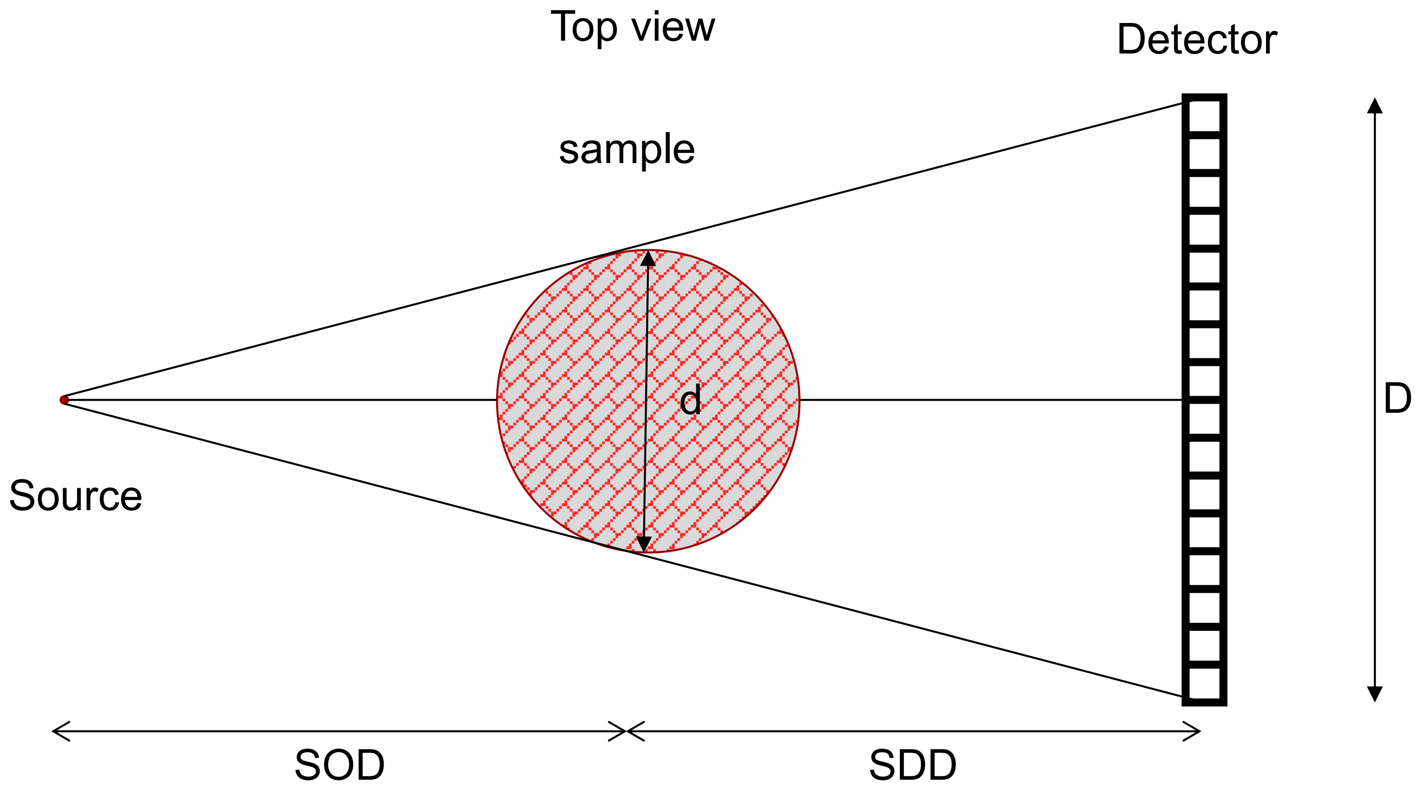

Figure by: E. Maire & P. J. Withers (2014) Quantitative X-ray tomography, InternationalMaterials Reviews, 59:1, 1-43, DOI: 10.1179/1743280413Y.0000000023

# Example of X-ray source for medical use

# X-ray Imaging or planar Xray imaging

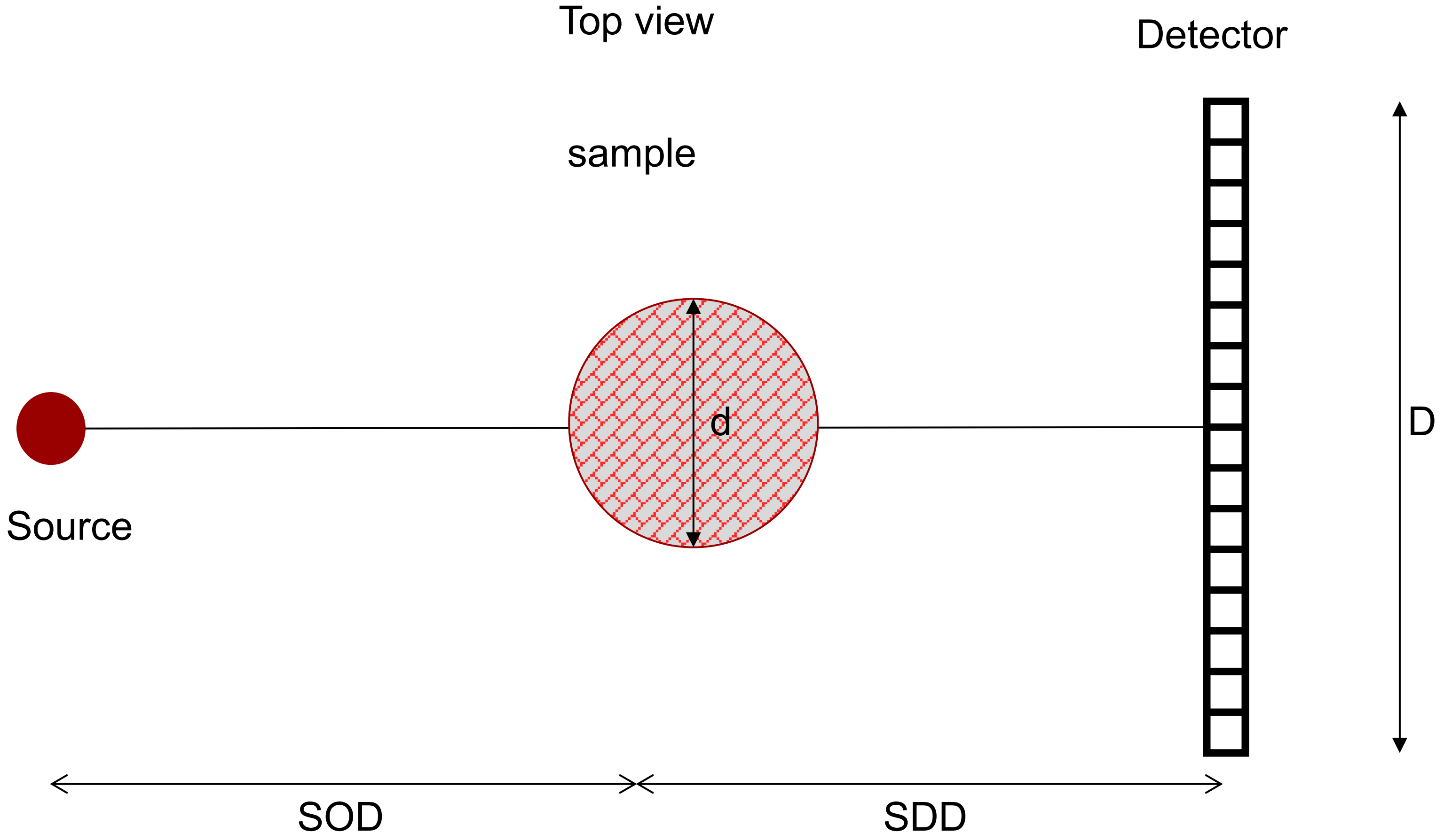
# Geometry and magnification

D = detector size
d = sample size
FOD = distance from source to object
SDD = distance from source to detector
M = magnification
dis = pixel to pixel distance/pixel pitch
vs = efficient pixel size

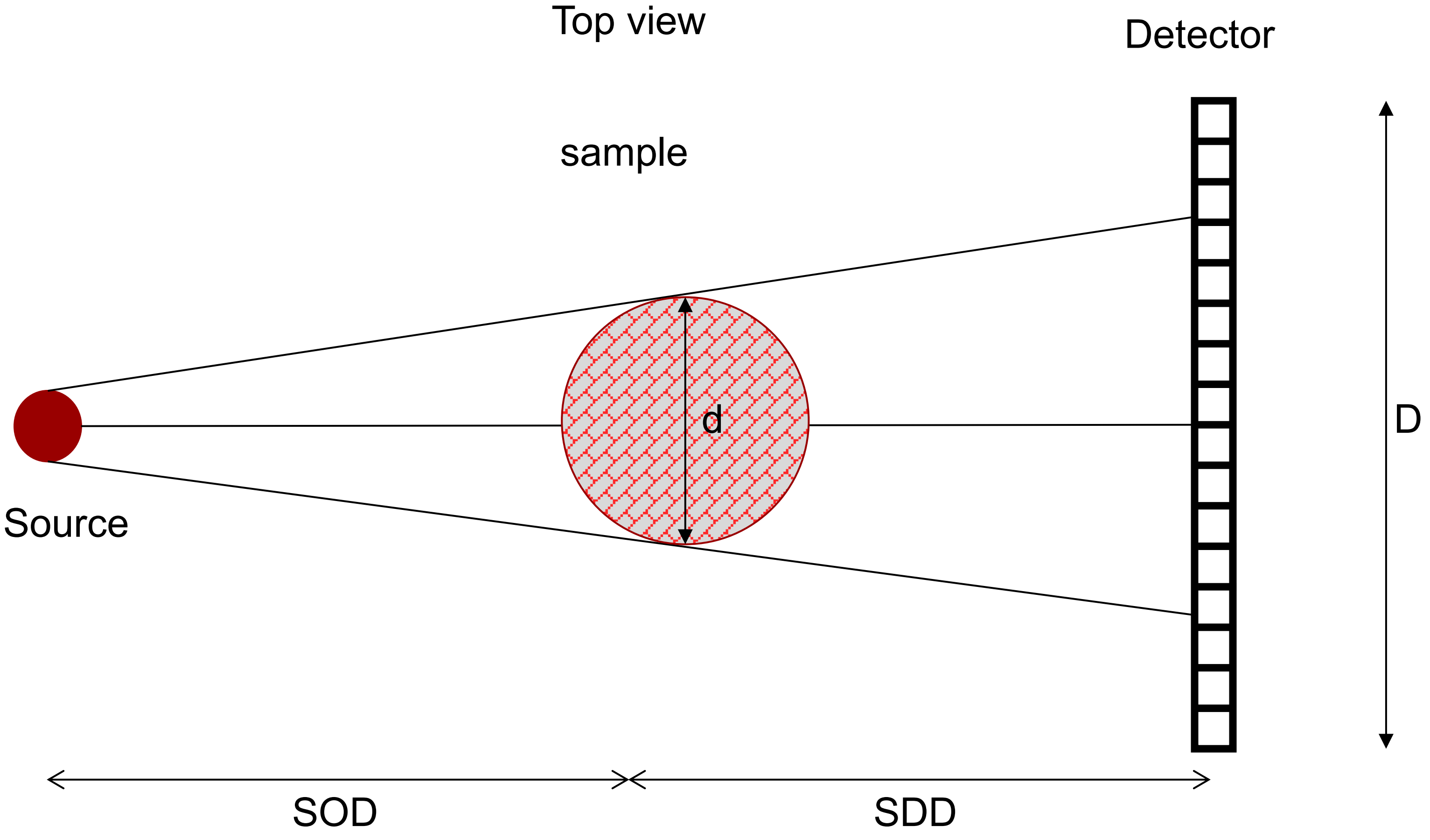



$$M = \frac{SDD + SOD}{SOD} \quad M_{Max} = \frac{D}{d} \quad vs = \frac{dis}{M}$$

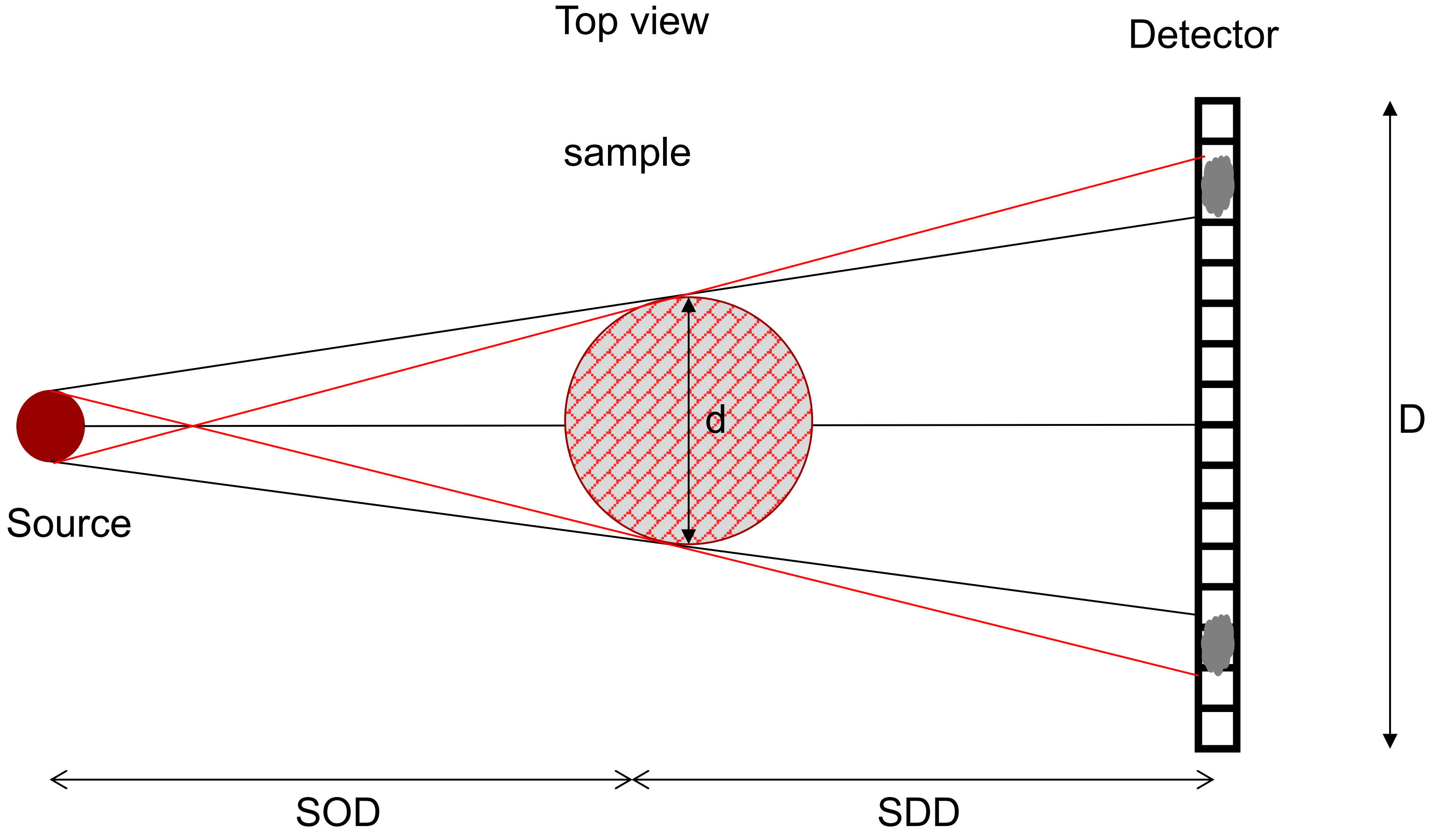
# Spot size and blurring effect



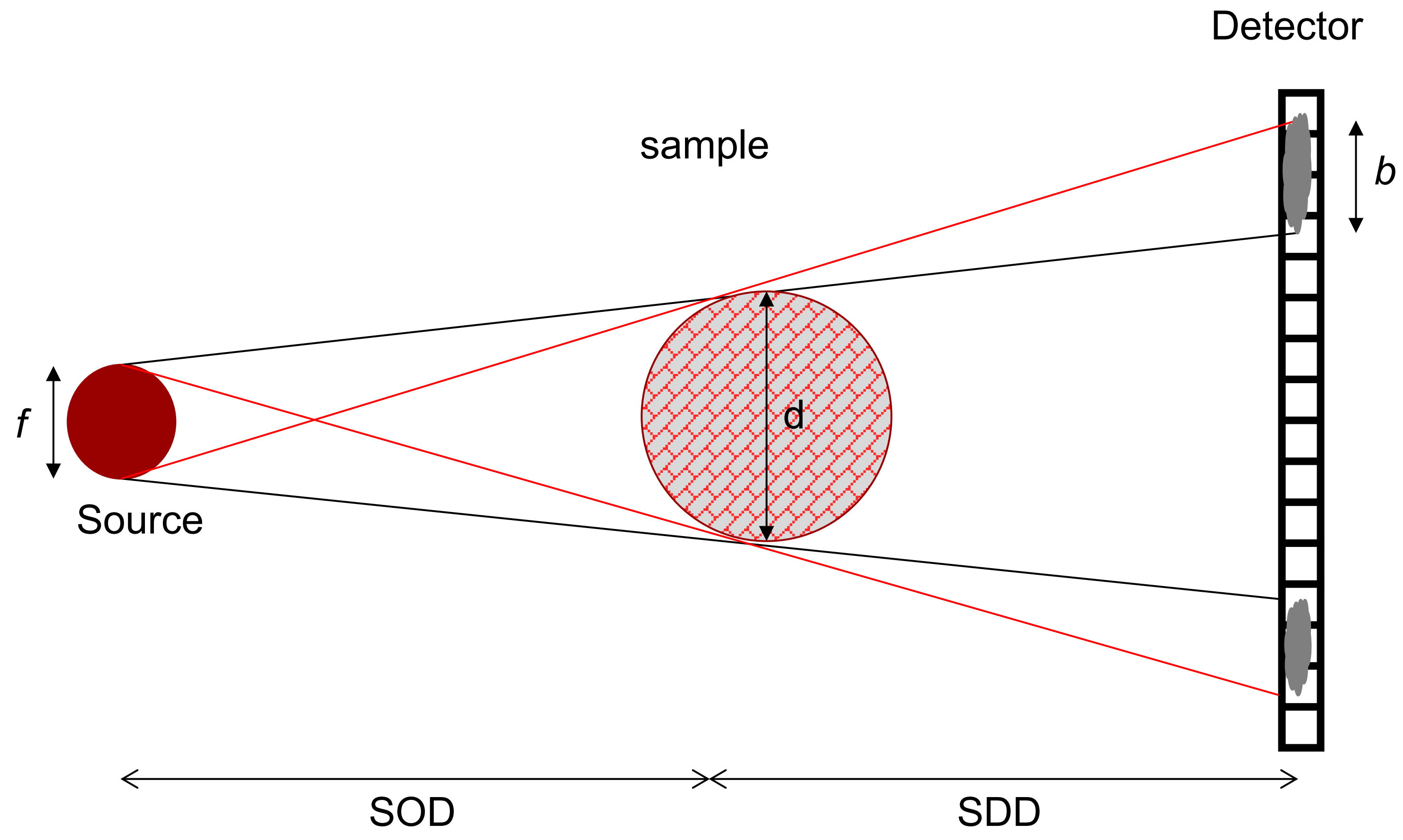
# Spot size and blurring effect



# Spot size and blurring effect



# What if the pixel size is smaller than the blurring effect of a large spot?




$$\frac{f}{SOD} = \frac{b}{SDD}$$

Magnification, *M:*

$$M = \frac{SDD + SOD}{SOD}$$

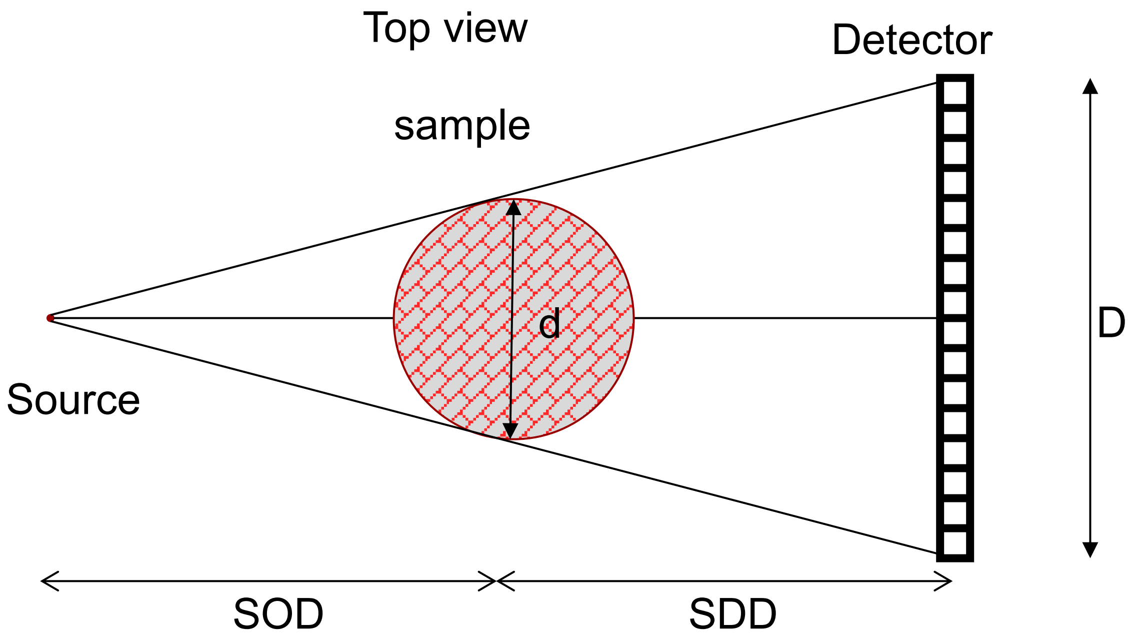
⇕

$$b = f(M-1)$$

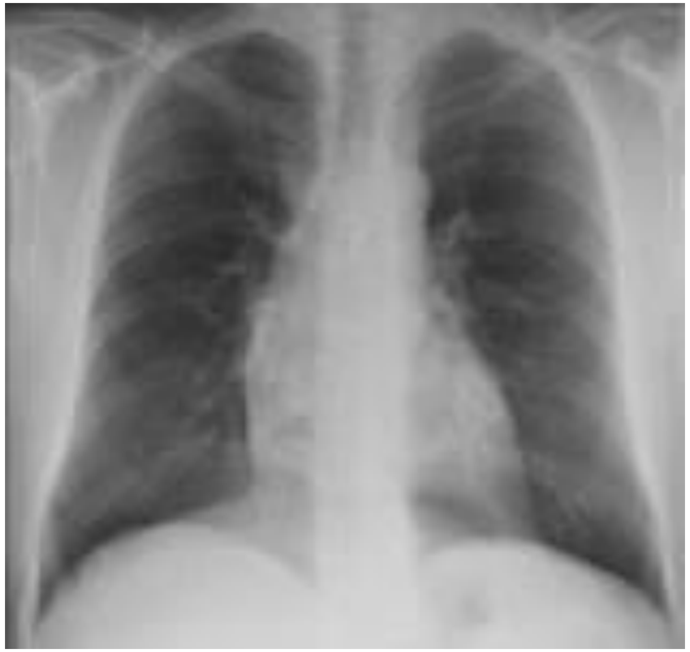
The image resolution is limited by the blurring effect

# Planar X-ray Imaging basics

- Projection imaging where the objects har absorbing X-rays (shadowing) before the detector.
- Images are ‘inverted’
  - White areas comes from material with high attenuation such as bone or metals
  - Black areas comes from material with low attenuation such as tissues and air
- Geometric magnification
  - Distance from source to object
  - Distance from object to detector



# Examples of medical X-ray images



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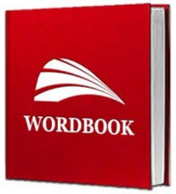
# We are not done with this lecture, but let's take a break

# X-ray interaction with matter

# Attenuation



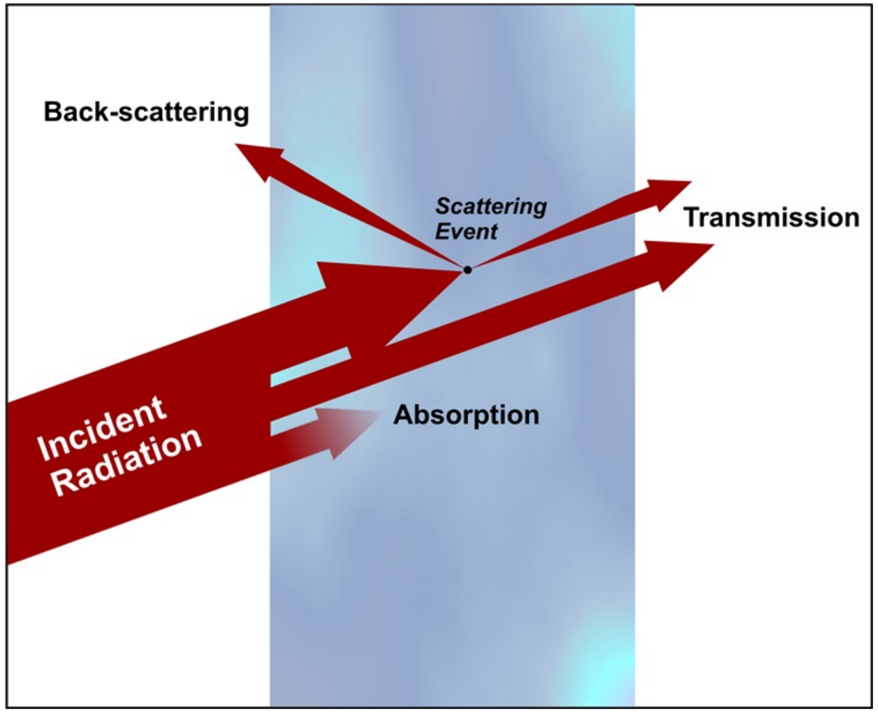

Attenuation means **“the reduction” of something**.
For example the reduction of the intensity of a signal.

**Attenuation is the sum of scattering and absorption**

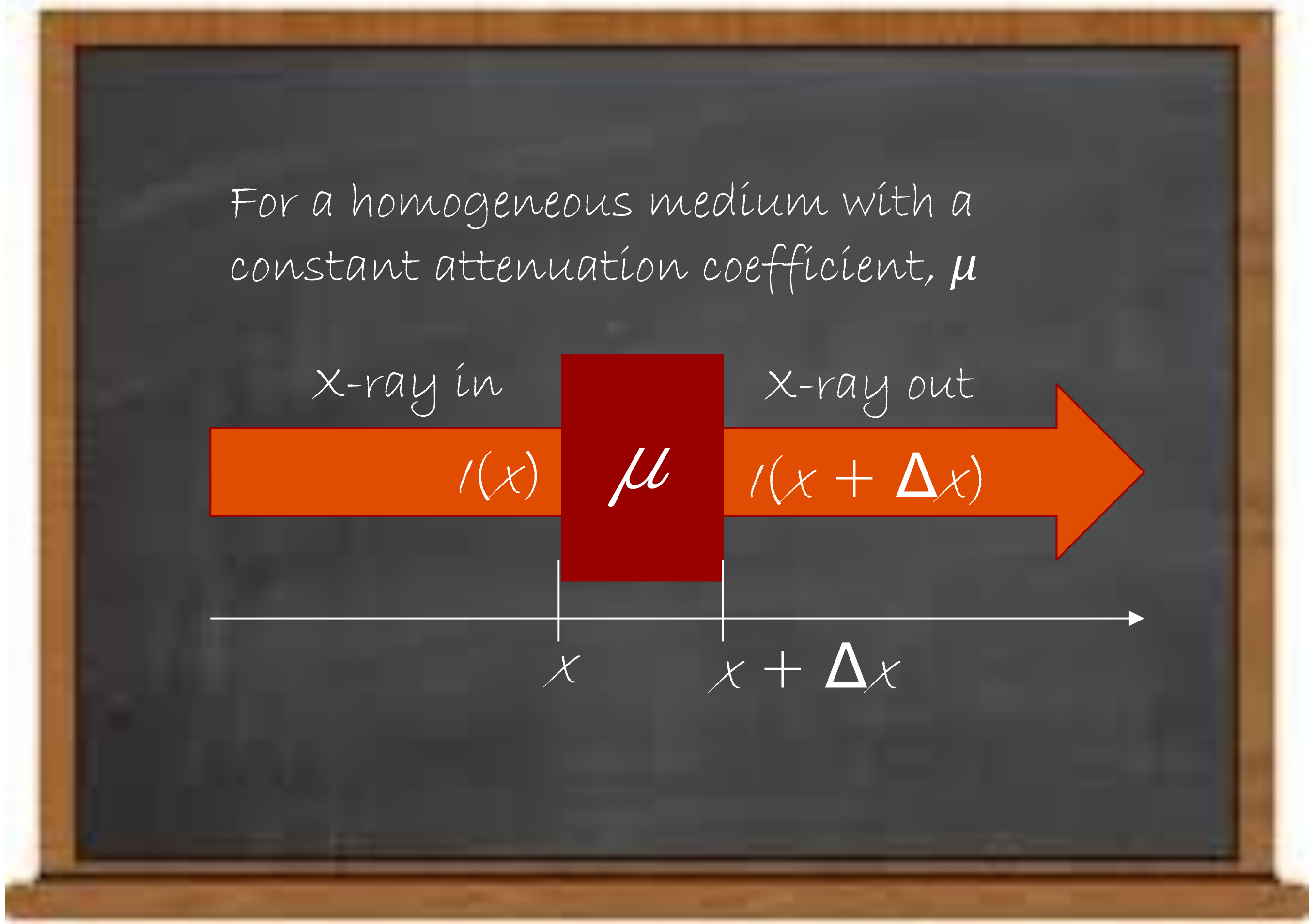
$\mu = \mu_s + \alpha$ (Unit = 1/m)

$\mu_s$ = scatter coefficient

$a$ = absorption coefficient



# Beer-Lamberts law



# Beer-Lamberts law

$$I(x+\Delta x) = I(x) - \mu I(x)\Delta x$$

$\Updownarrow$

$$\frac{I(x+\Delta x) - I(x)}{\Delta(x)} = -\mu I(x)$$

$\Updownarrow$

$$\lim_{\Delta x \to 0} \frac{I(x+\Delta x) - I(x)}{\Delta(x)} = \frac{dI}{dx} = -\mu I(x)$$

$\Updownarrow$

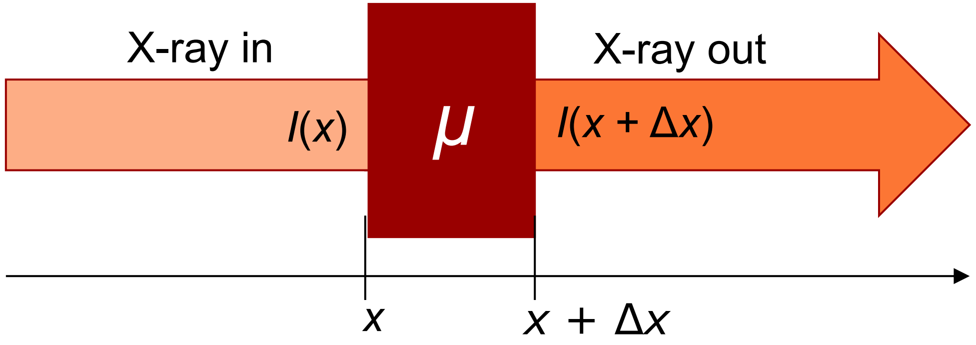
$$\int \frac{dI}{I(x)} = -\mu \int dx$$

$\Updownarrow$

$$\ln\big(I(x)\big) = -\mu x + C$$

$\Leftrightarrow$

For a homogeneous medium with a constant attenuation coefficient, $\mu$



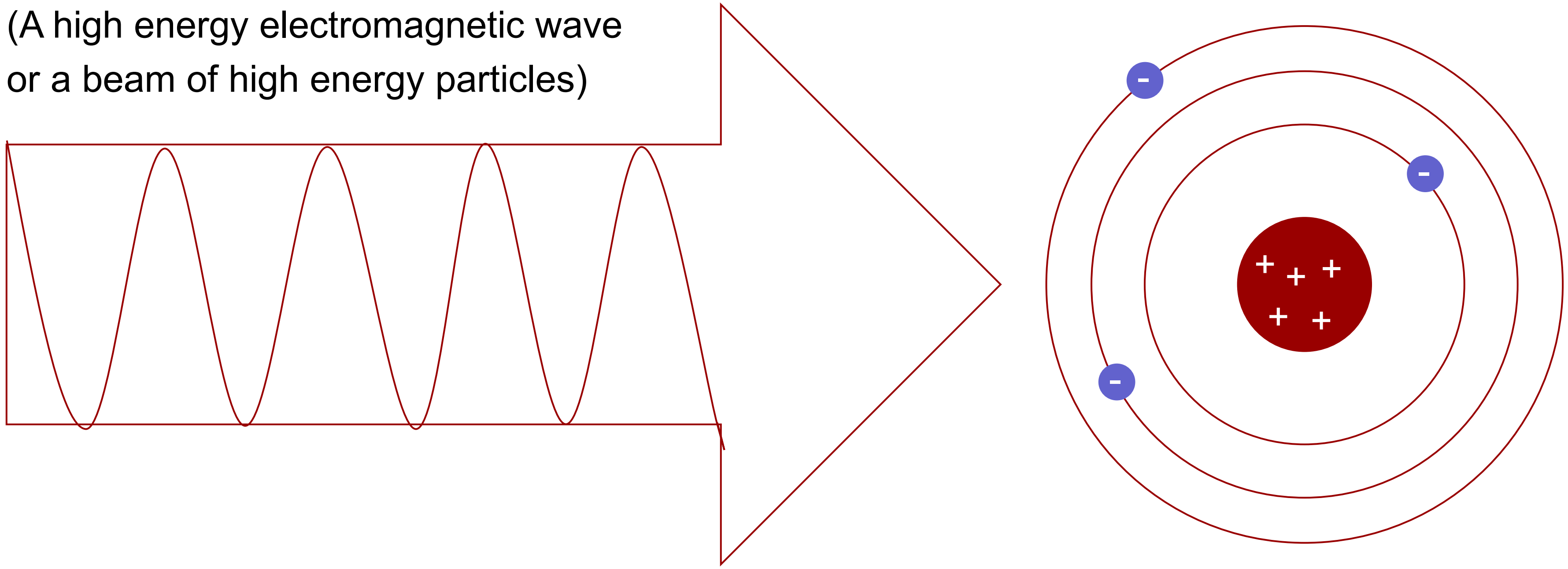

$$I(x) = I_0 e^{-\mu x}$$

$I_0$ = initial intensity

# What are the mechanisms for attenuation?

**Think about x-rays ……………………………………………………..... hitting an atom**

(A high energy electromagnetic wave
or a beam of high energy particles)

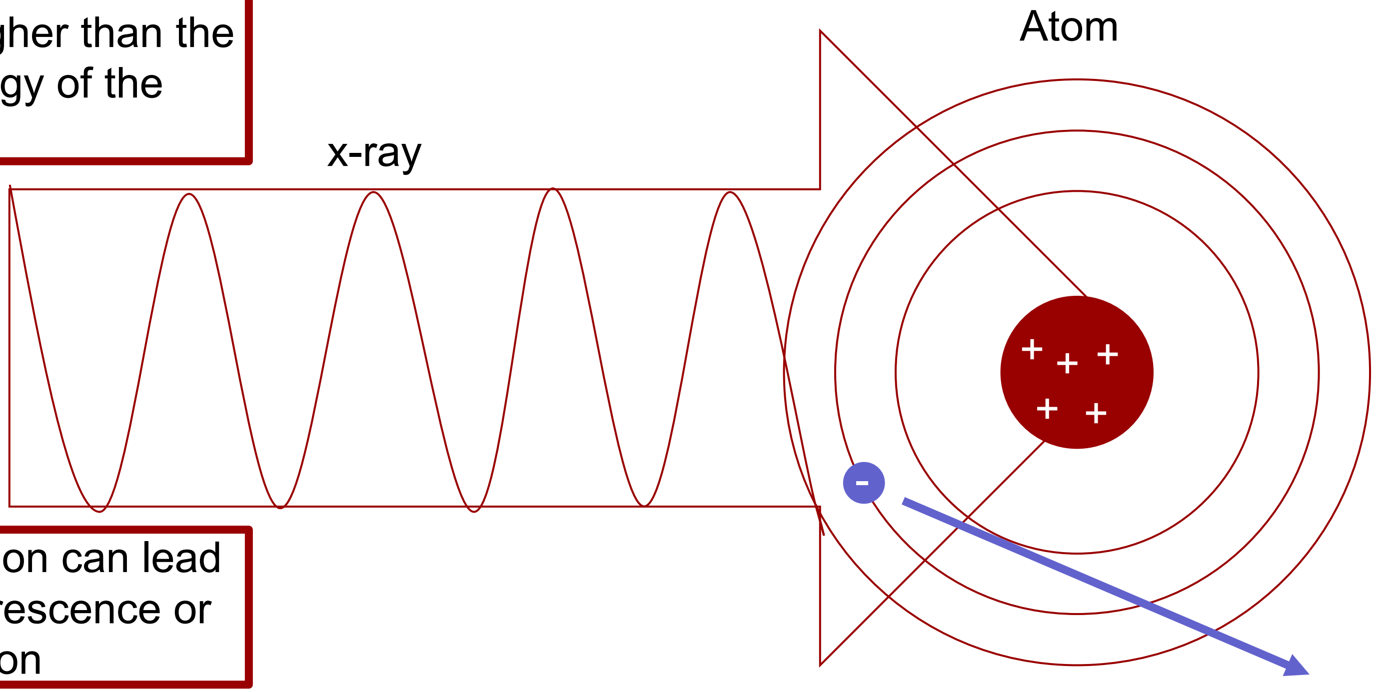


What kind of x-ray-atom interactions can you imagine?
Discuss this in your group for 5 min

# Mechanisms of attenuation: Photoelectric Absorption

$$\alpha = k \frac{\rho}{A} \frac{Z^4}{(h\omega)^3}$$

The x-ray can only kick out the electron if its energy is higher than the binding energy of the electron!




Recombination can lead to x-ray fluorescence or Auger electron

$k$ is a constant that depends on the shell involved

$\rho$ is the density

$A$ is the atomic weight

$h$ is Planck constant

$\omega$ is the photon frequency

$Z$ is the atomic number

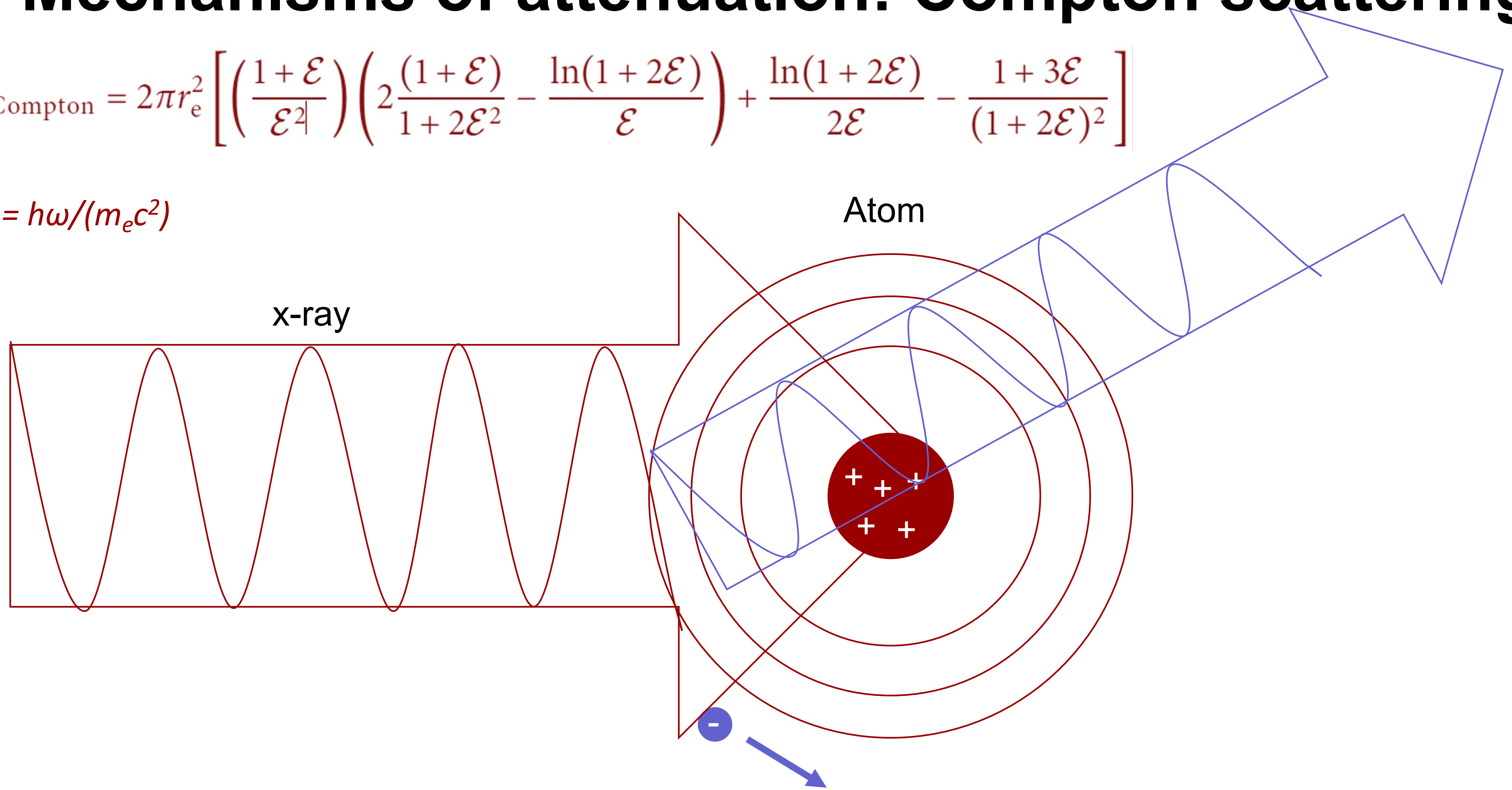
Notice the strong dependence on Z

The electron of a lower shell is kicked off the atom and travels through the material as a free photoelectron

# Mechanisms of attenuation: Compton scattering

$$\sigma_{\mathrm{Compton}} = 2\pi r_e^2 \left[ \left( \frac{1+\mathcal{E}}{\mathcal{E}^2} \right) \left( 2\frac{(1+\mathcal{E})}{1+2\mathcal{E}^2} - \frac{\ln(1+2\mathcal{E})}{\mathcal{E}} \right) + \frac{\ln(1+2\mathcal{E})}{2\mathcal{E}} - \frac{1+3\mathcal{E}}{(1+2\mathcal{E})^2} \right]$$

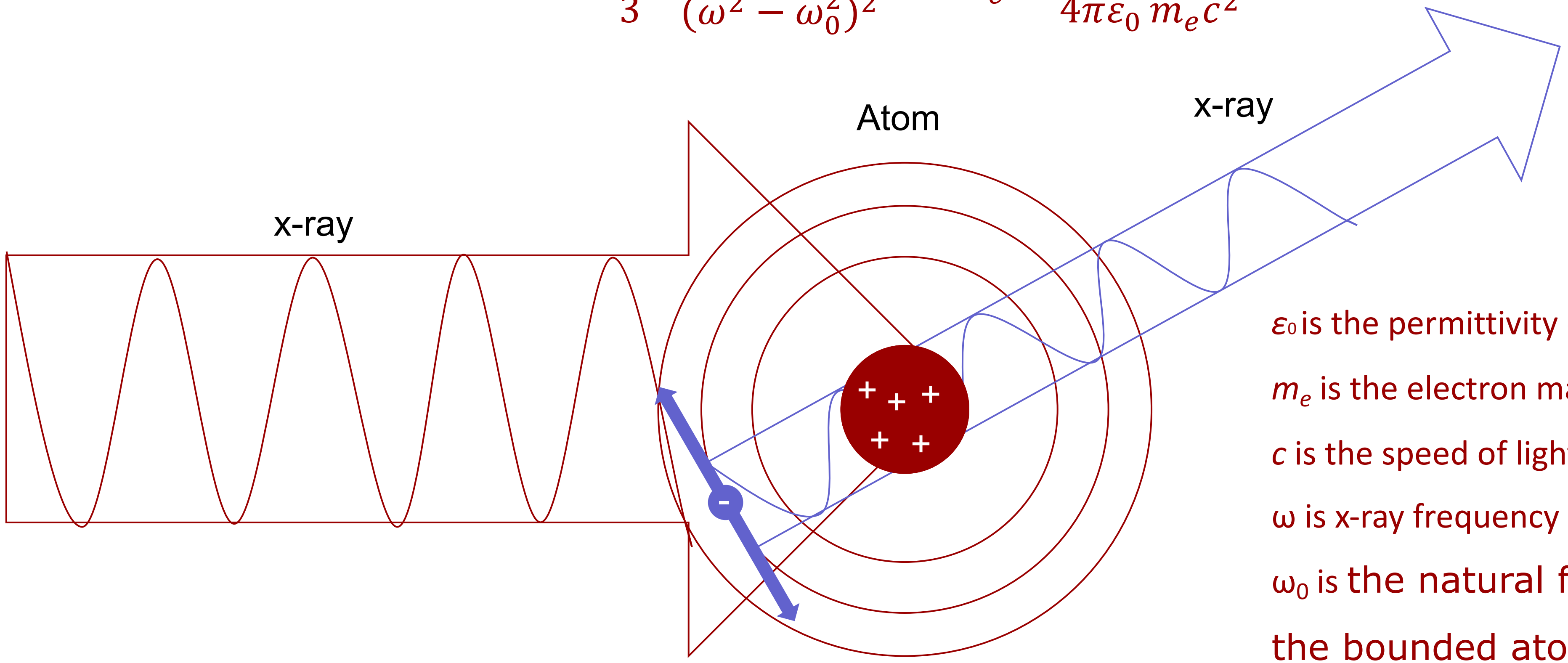
$\varepsilon = h\omega/(m_e c^2)$




The x-ray kicks out a quasi-free electron and looses some of it's energy

# Mechanisms of attenuation: Rayleigh or Thomson scattering

$$\sigma = \frac{8\pi r_e^2}{3}\frac{\omega^4}{(\omega^2 - \omega_0^2)^2} \qquad r_e = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{m_e c^2}$$




$\varepsilon_0$ is the permittivity of free space

$m_e$ is the electron mass

$c$ is the speed of light

$\omega$ is x-ray frequency

$\omega_0$ is the natural frequency of the bounded atom electrons

The electric field of the incoming beam drives strongly bound electrons up and down. This makes the electrons radiate

# Mechanisms of attenuation: Pair production

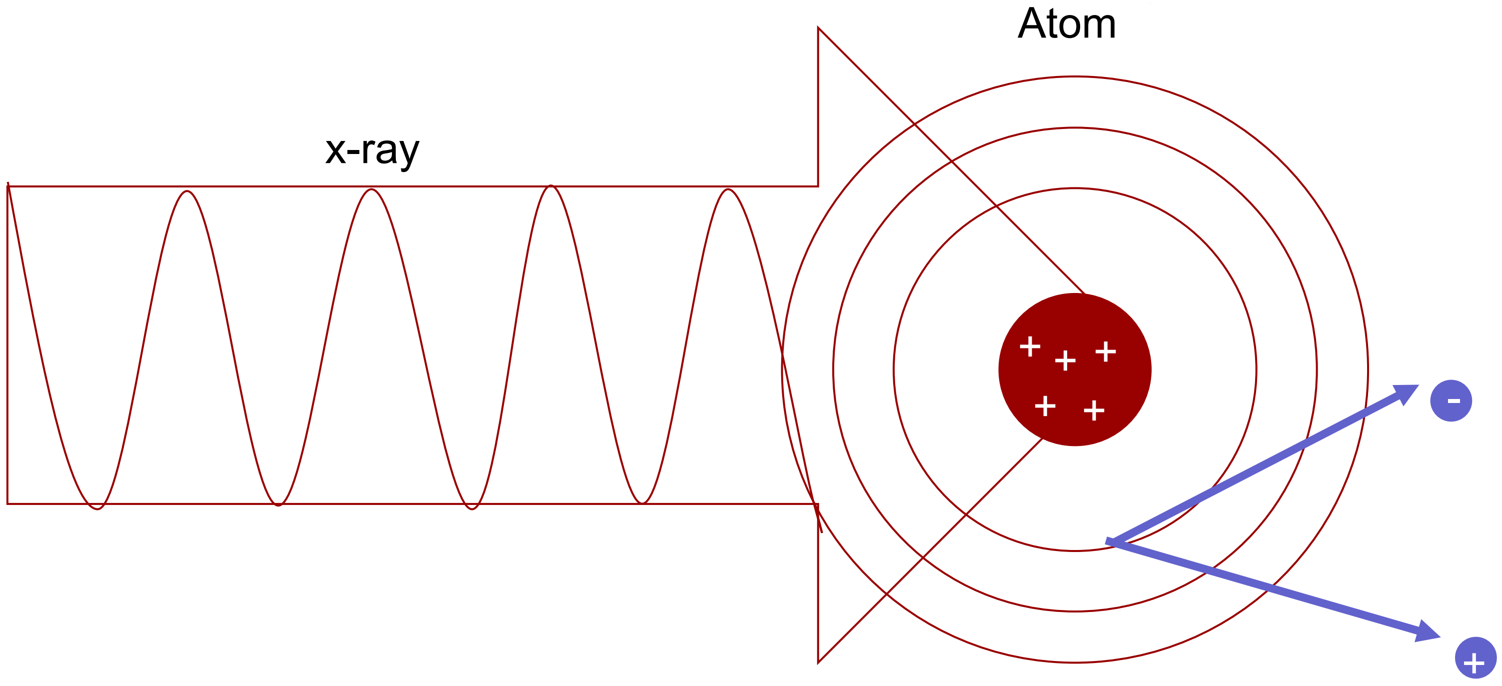
$$\sigma_{\text{pair production}} = \alpha r_e^2 Z^2 \left[ \frac{28}{9} \ln(2\mathcal{E}) - \frac{218}{27} + \frac{6.45}{\mathcal{E}} \right]$$

$\alpha$ is a fine-structure constant

$\varepsilon = h\nu/(m_e c^2)$

$Z$ = atomic number

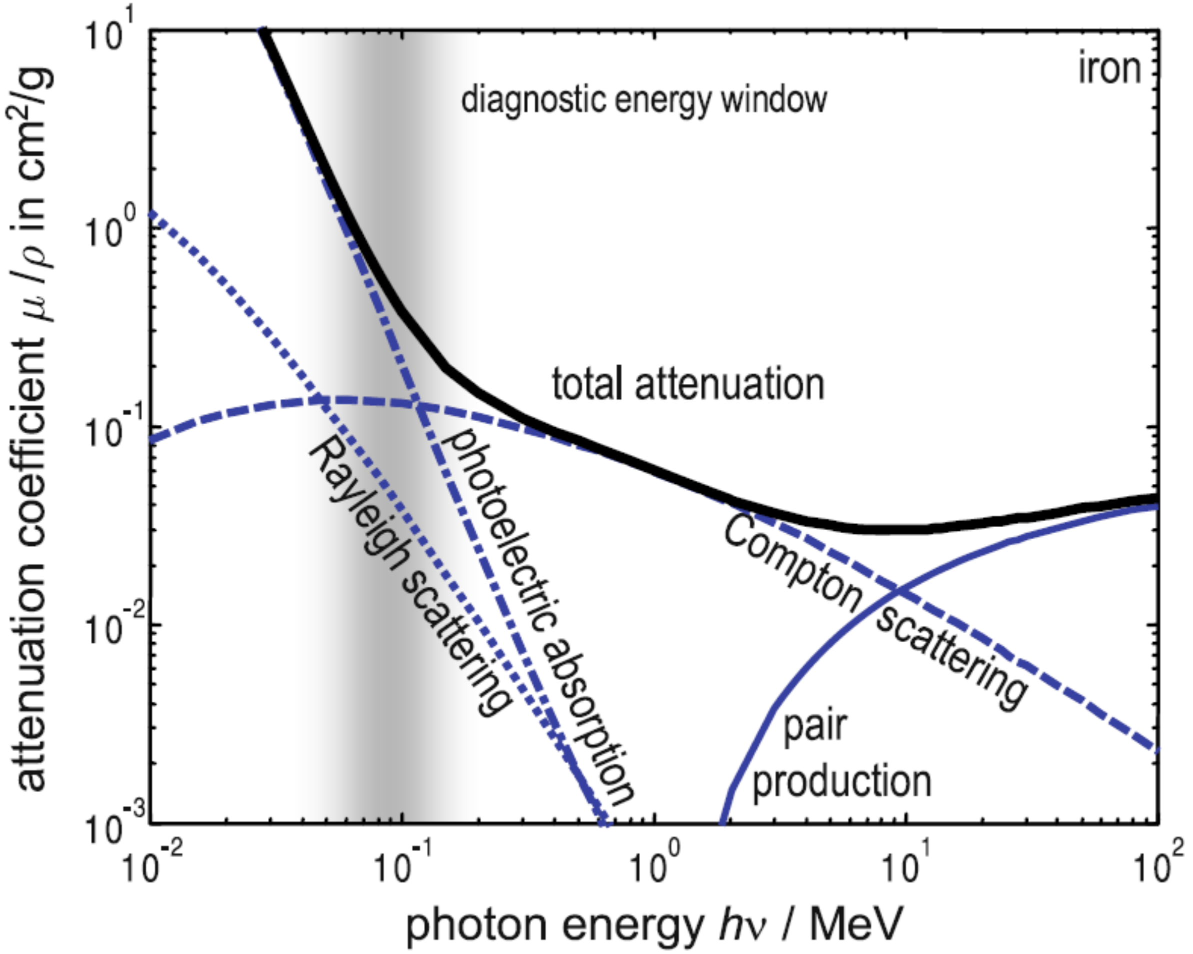
$$r_e = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{m_e c^2}$$

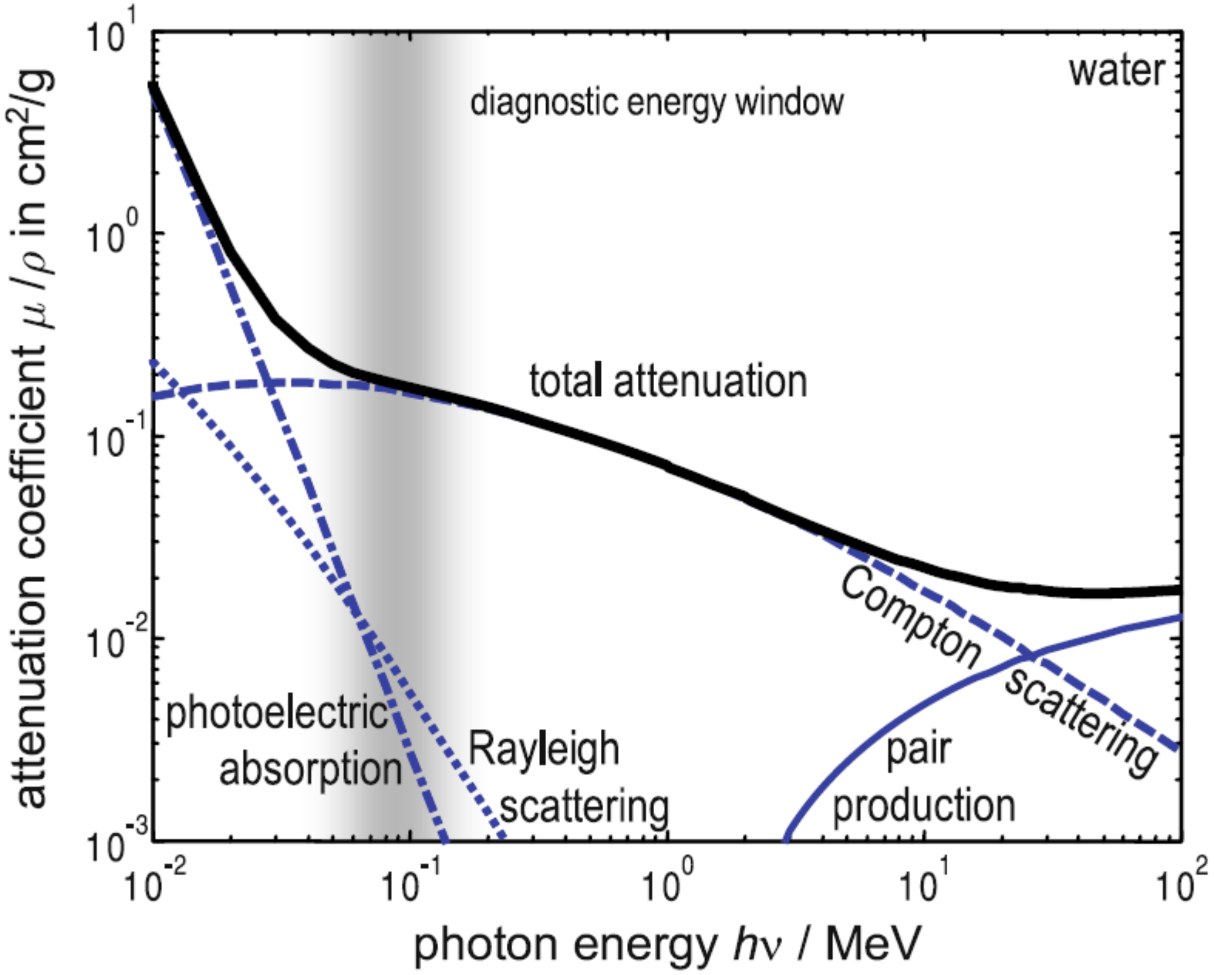



For high energy x-ray (gamma rays) the x-ray energy can be used for production of antiparticles.

$$photoelectric\ absoption:\ \alpha = k\frac{\rho}{A}\frac{Z^4}{(h\omega)^3}$$

# How much does each mechanism contribute?

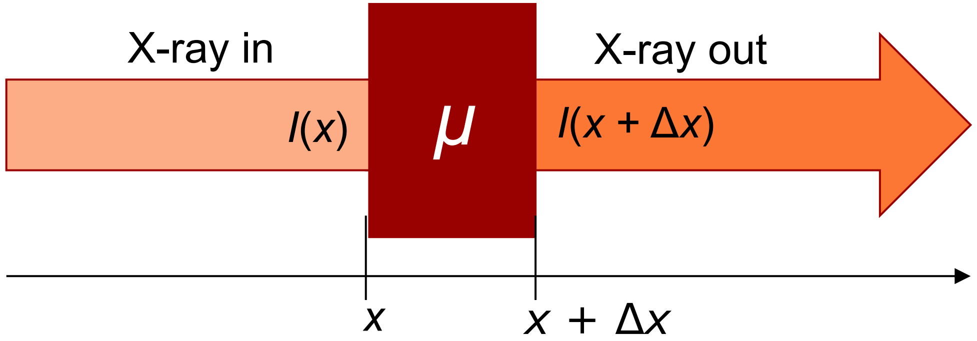



Reference: Thorsten M. Buzug Computed Tomography

# Absorbtion

For a homogeneous medium with a constant attenuation coefficient, $\mu$




$$I(x) = I_0 e^{-\mu x}$$

$I_0$ = initial intensity

$$absorption \propto \frac{Z^4}{\mathcal{E}^3}$$

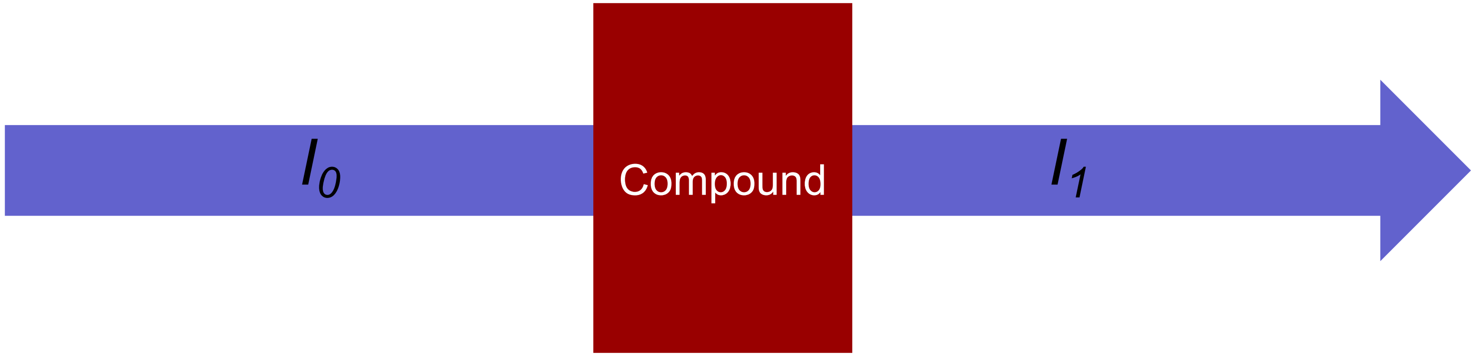
| absorption | 12 keV | 30 keV | 70 keV | 150 keV | 225 keV |
|---|---|---|---|---|---|
| Air (1m) | 30% | 0% | 0% | 0% | 0% |
| Aluminium (1mm) | 98,2% | 26,1% | 6,1% | 3,7% | 3,2% |
| Iron (1mm) | 100% | 99,8% | 47,0% | 14,2% | 10% |
| Lead (1mm) | 100% | 100% | 97,8% | 89,6% | 57,5% |

# Mass attenuation coefficient $\mu/\rho$

| | 50 keV | 100 keV | 200 keV |
|---|---|---|---|
| Air | 0,208 | 0,154 | 0,122 |
| Water | 0,227 | 0,171 | 0,137 |
| Fat | 0,212 | 0,169 | 0,136 |
| Musle | 0,226 | 0,169 | 0,136 |
| Bone | 0,424 | 0,186 | 0,131 |
| Lead | 8,041 | 5,549 | 0,999 |

Data from http://physics.nist.gov/PhysRefData/XrayMassCoef/cover.html

# Complex materials - compounds




Imagine that the material is structurally homogeneous (for example no pores), but it is a compound (not just composed of a single element. Can we still use the Beer-Lambert law?

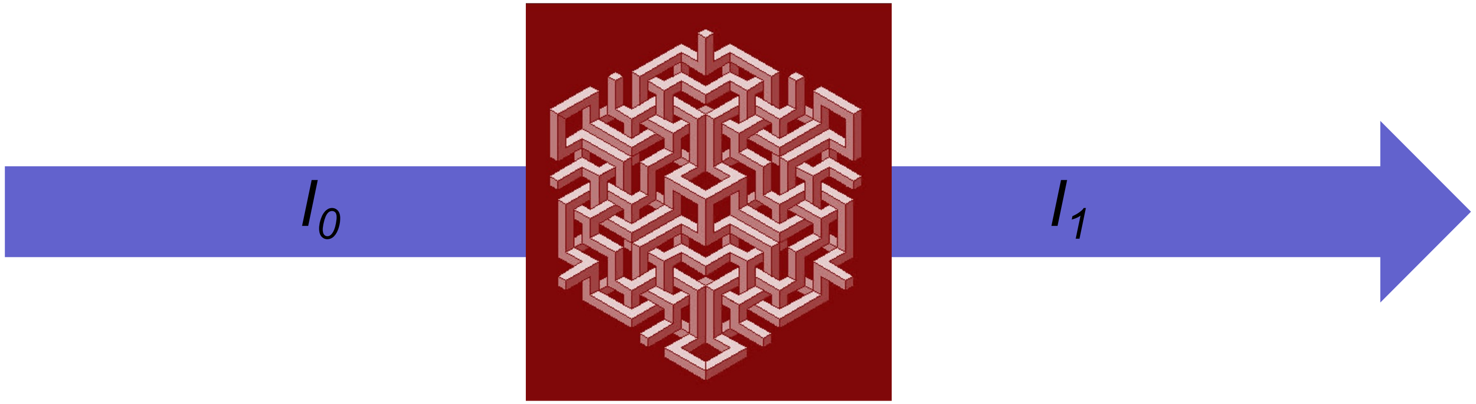
Yes: We can use a weighted average of μ for each element

Example: Au-Ni alloy with 10 % Au.

For an x-ray energy of 100 keV the attenuation coefficients are: Au = 100 $cm^{-1}$, Ni = 4 $cm^{-1}$

The effective attenuation coefficient for the alloy at 100 keV = 0.1 x 100 $cm^{-1}$ + 0.9 x 4 $cm^{-1}$ = 14 $cm^{-1}$

# Complex materials - compounds




Imagine that the material has structures (for pores). Can we still use the Beer-Lambert law?

Then $\mu$ becomes $\mu(x)$ and there is no simple solution to the differential equation

$$I(x) = I_0 e^{-\int \mu(x) dx}$$

We cannot solve this equitation just by one measurement of I(x) and $I_0$.

X-ray CT → Projections from many angles around the material

→ Many measurements of I(x) through the same points

→ Offer approximate solutions to the system of equations.

The more projection angles, the better the approximation.

DTU

# Beam hardening


What if the x-ray source produces a white beam (not monochromatic)? Can we still use the Beer-Lambert law?

We then include an integral over the energy range

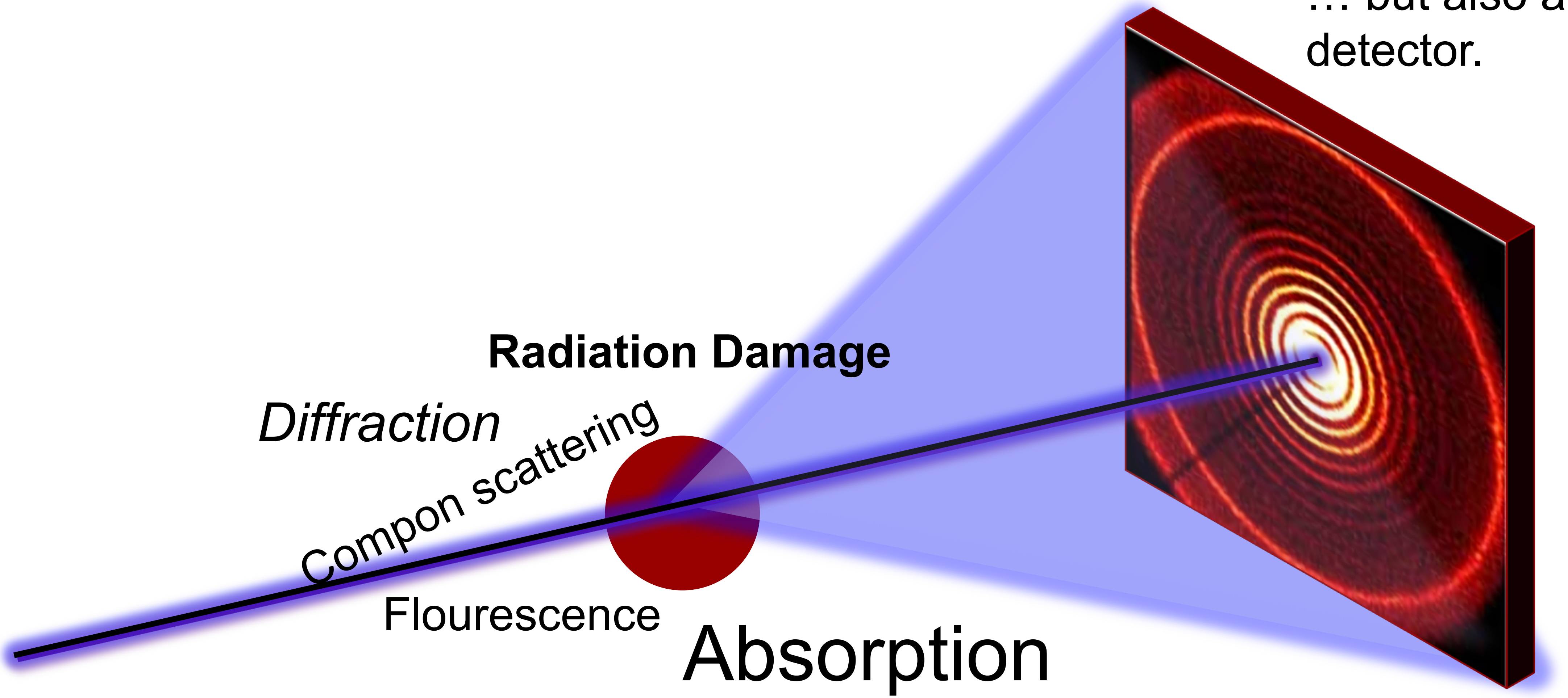
$$I(x) = \int I_0 e^{-\int \mu(x)dx}\, dE$$

In practice we ignore this. Although it will introduce an artefact in the CT data, the so-called **Beam hardening artefact**

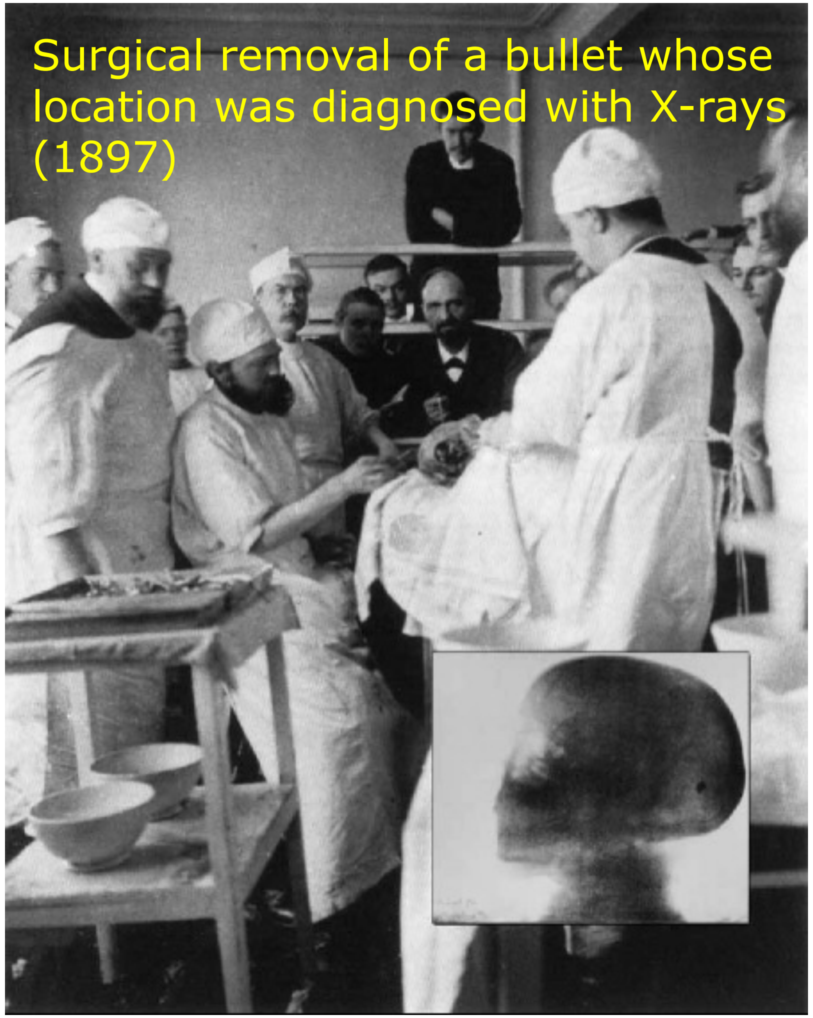
# X-ray detectors

# X – rays interactions

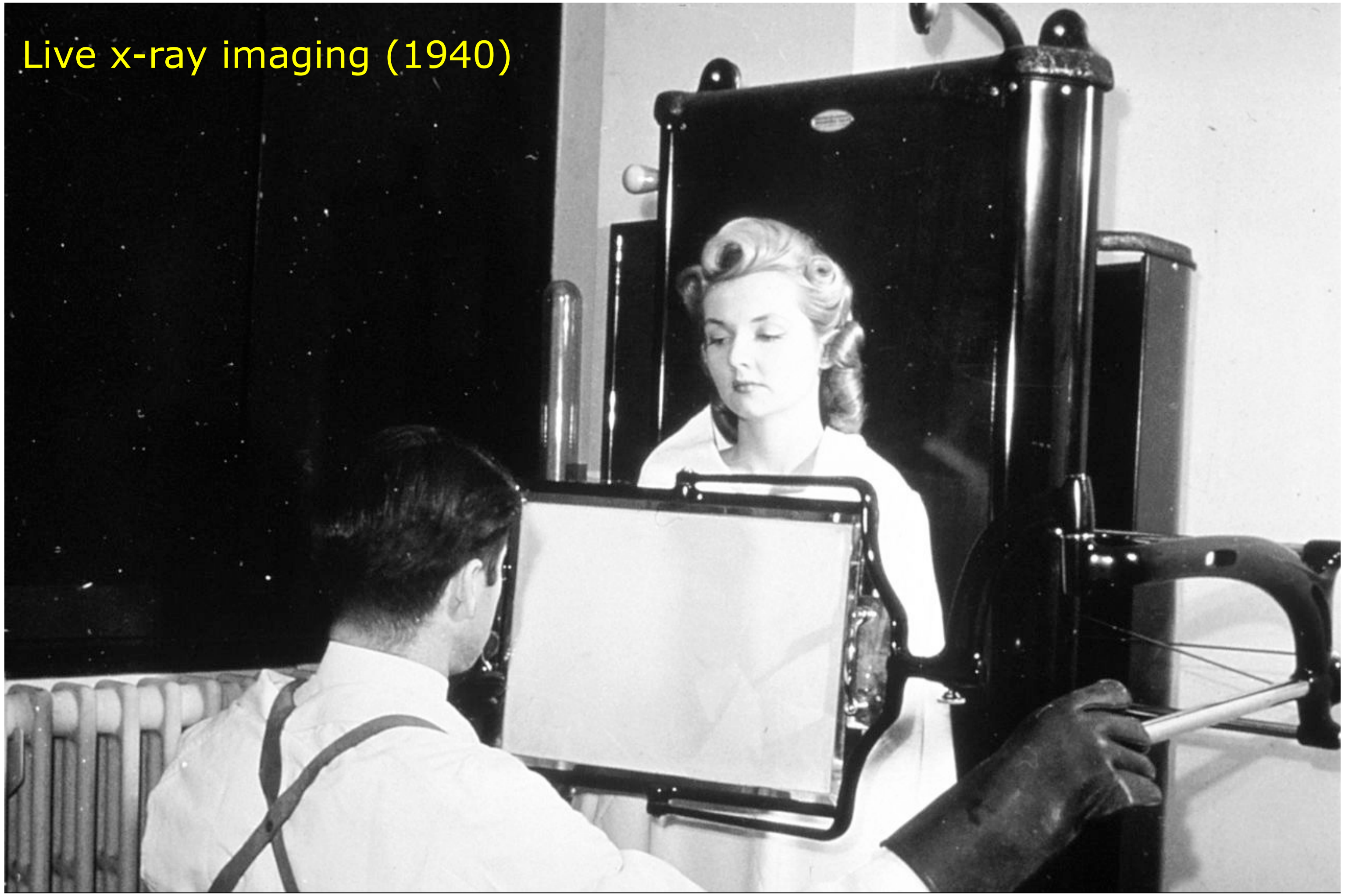
… but also at the detector.



# Early medical applications

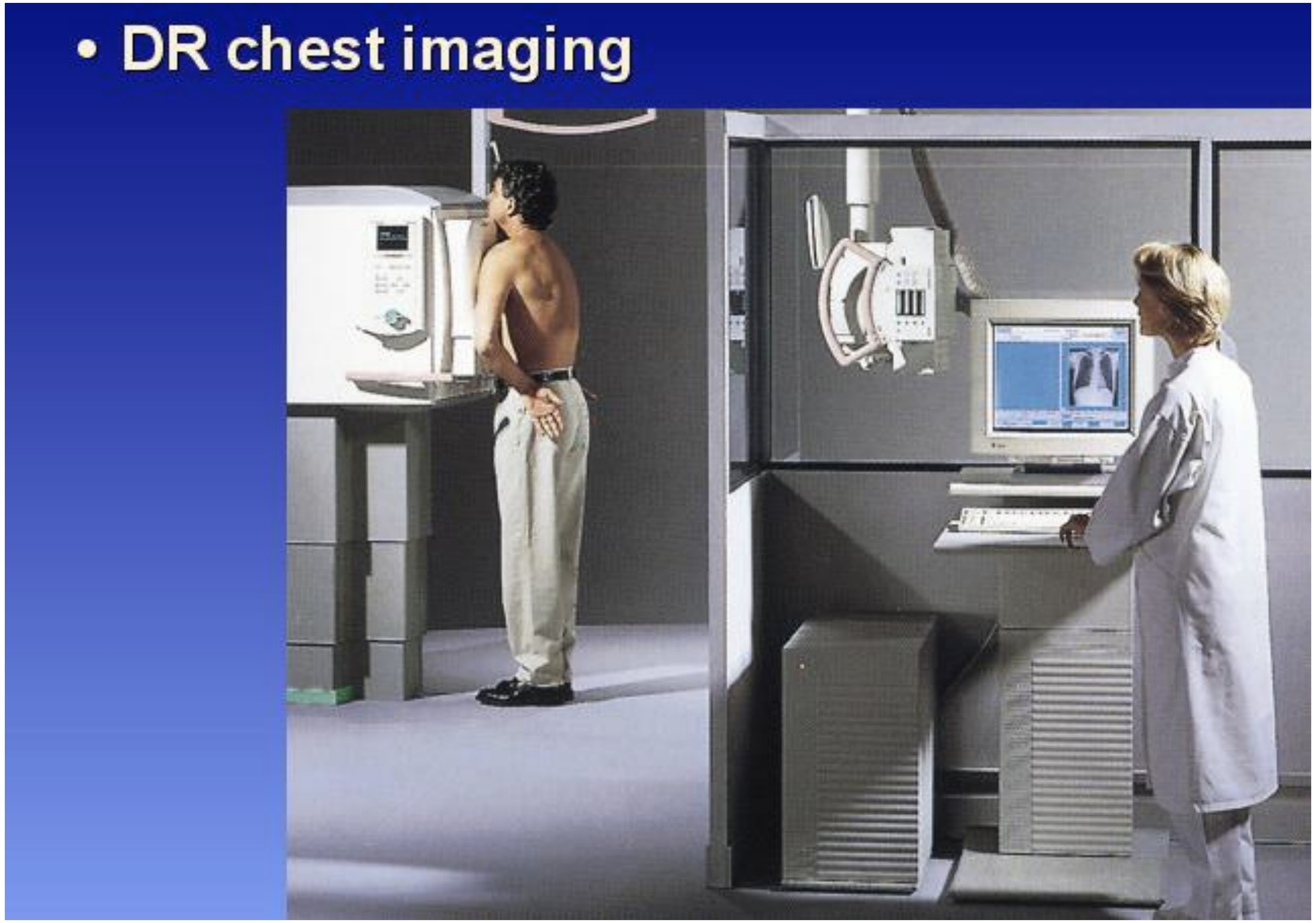


Surgical removal of a bullet whose location was diagnosed with X-rays (1897)



Live x-ray imaging (1940)

# Digital radiology



# X-ray Detectors

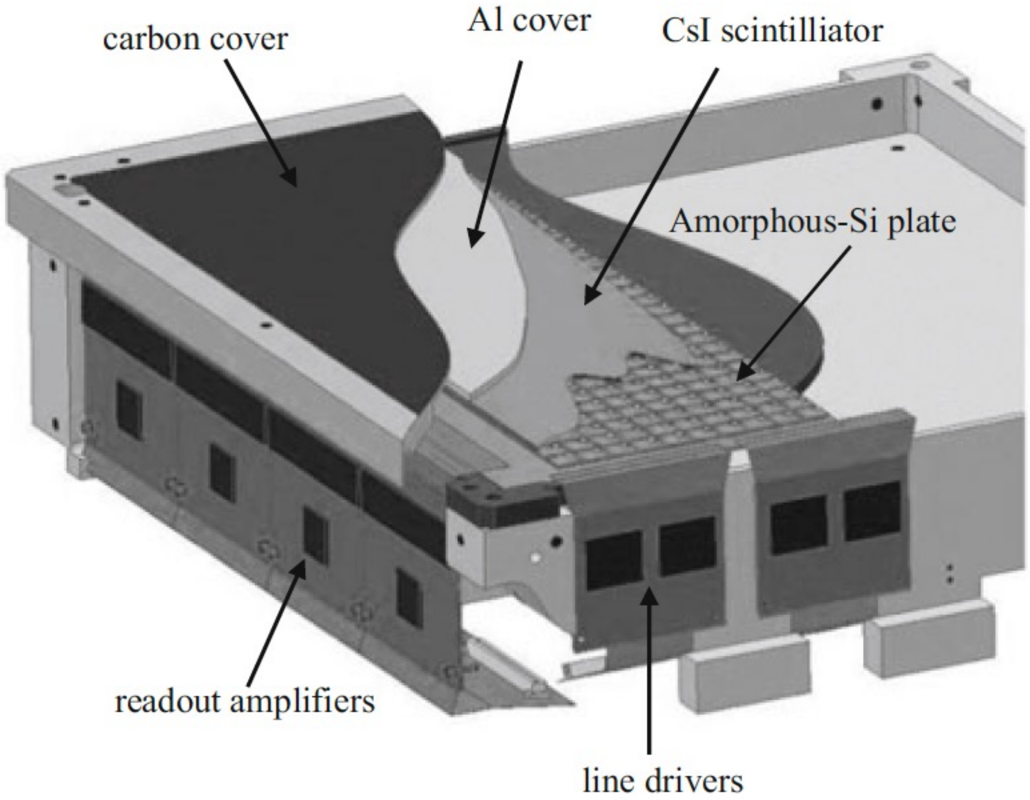
Photon Interaction method

- Scintillating
- Solid state detectors

Signal processing Method

- Integrating
- Photon counting

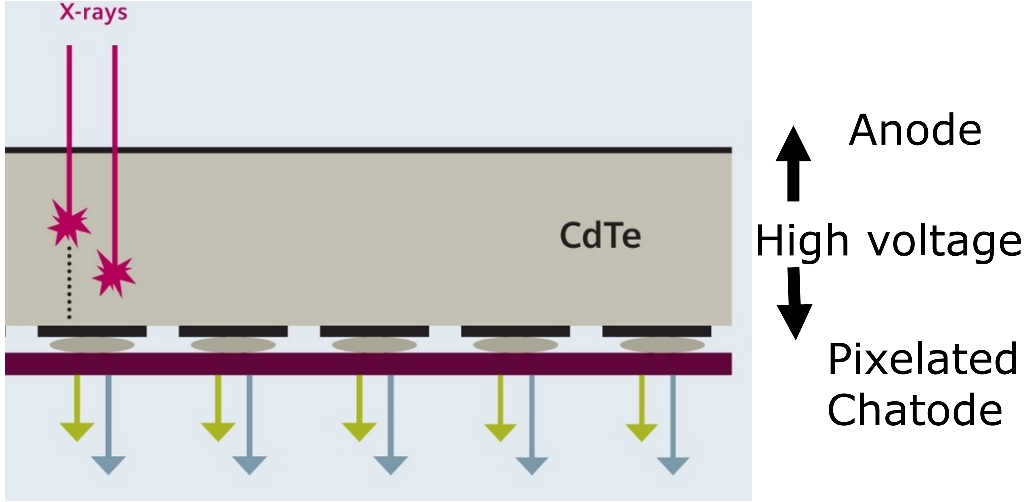

# Inside the flat panel

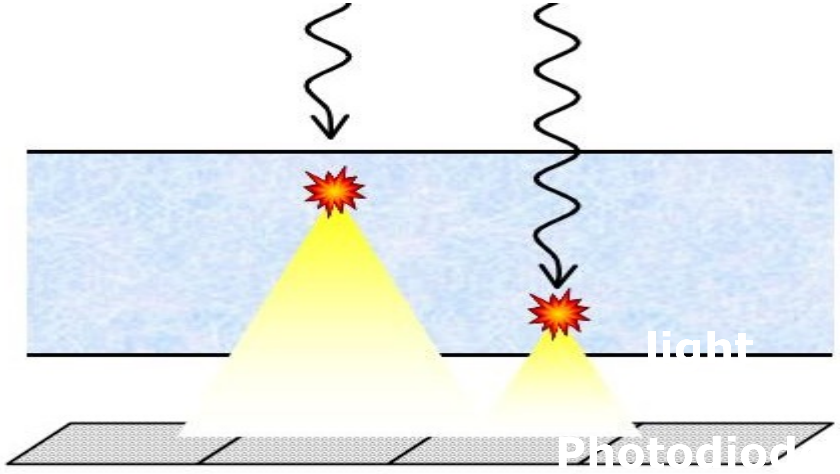



Curtesy: General Electric CT systems

# Photon interaction method

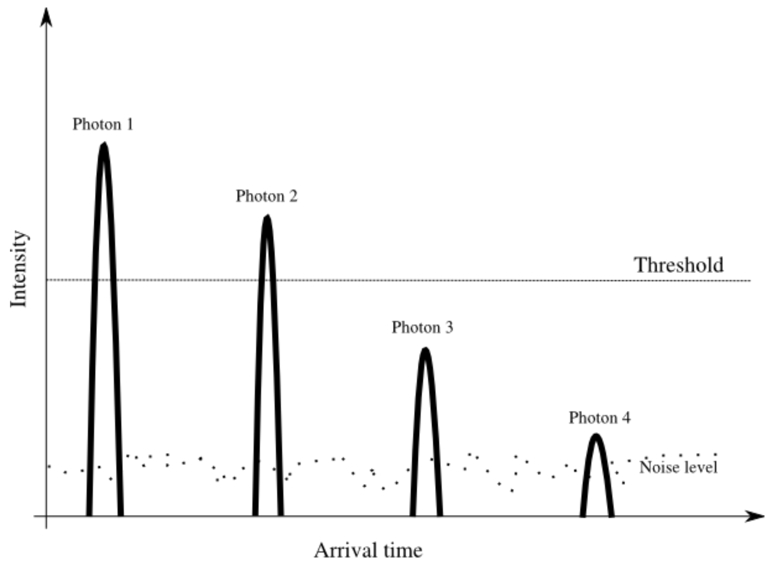

- Solid state
  - Silicon
  - Germanium
  - Cadmium Telluride
- Scintillator
  - Caesium Iodide
  - Lutetium Aluminum Garnet

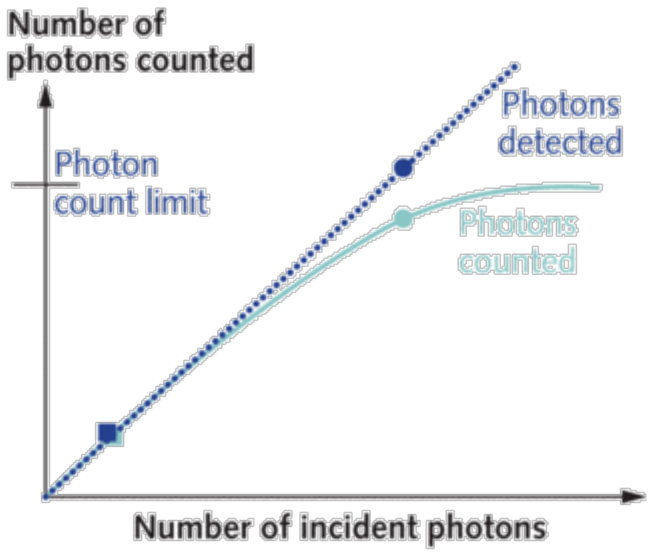


# Signal Processing method

- Integrating
- Photon counting

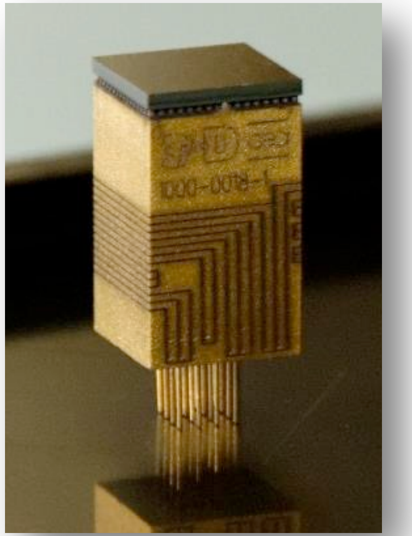


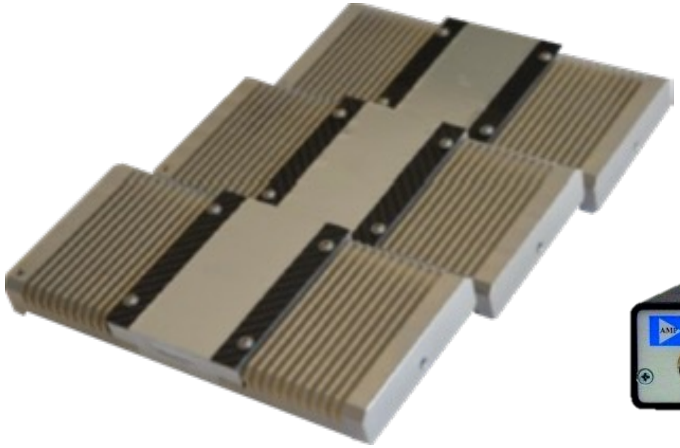




Photon count limit 5e8 photons pr second pr pixel

# Spectral Detectors

Collaborating and working with
- Advacam
  - 2D based on Timepix
  - Simultanous ToT and ToA
- CEA Saclay
  - 2D based on Caliste architecture
  - Low power
- Multix
  - 1D LETi ASIC
  - Designed for high flux 1e7ph/mm^2/s
- Amptek
  - 0D
  - Energy resolution 0.8 keV



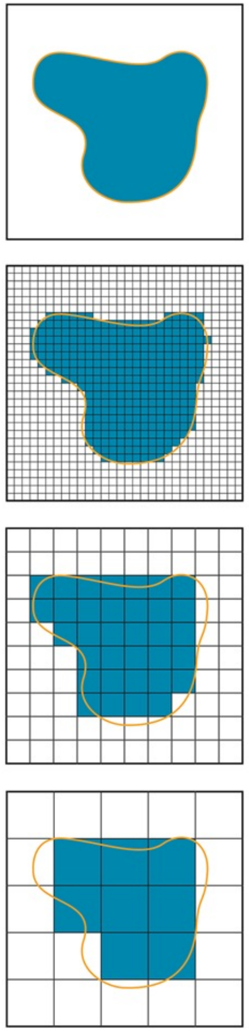
# Image resolution (or spatial resolution)

How would you define **spatial resolution**?

*How far two features need to be separated to be distinguishable in the image*

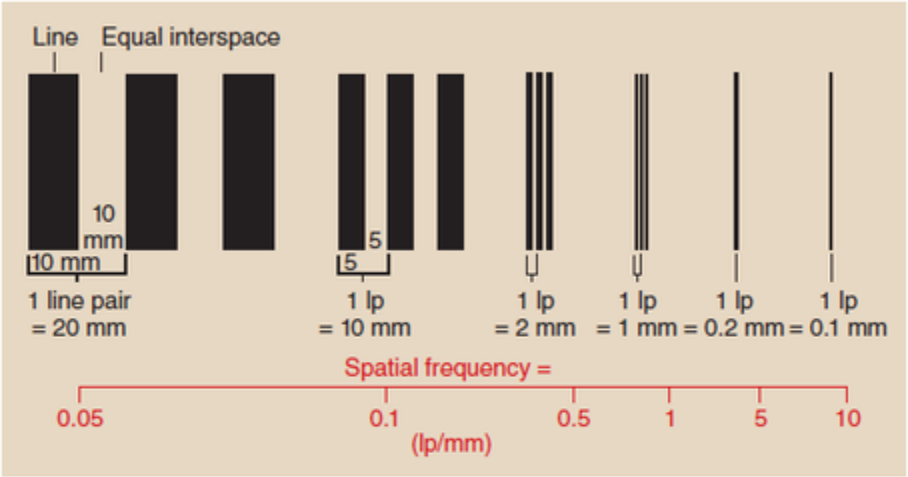
**Pixel resolution**

Pixel resolution is the size of the pixels in the image (not the physical size of the pixel in the detector)

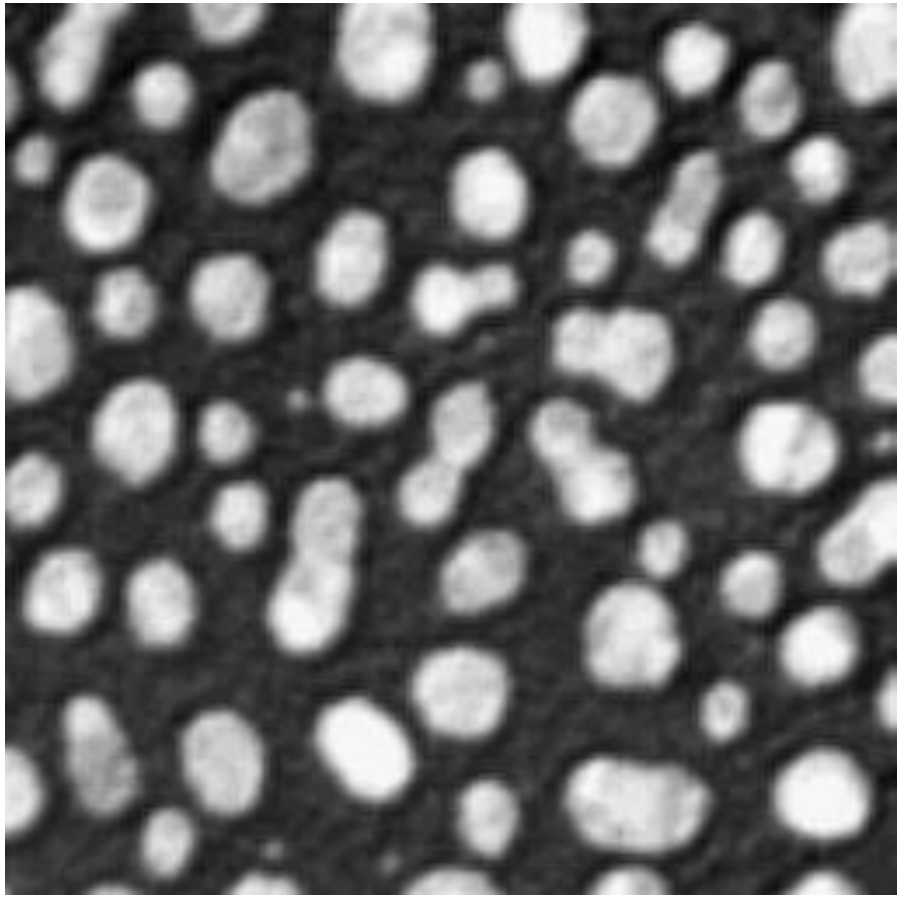


Lets say that we will record an image where the pixel size is 100 µm. Is the spatial resolution then also 100 µm?

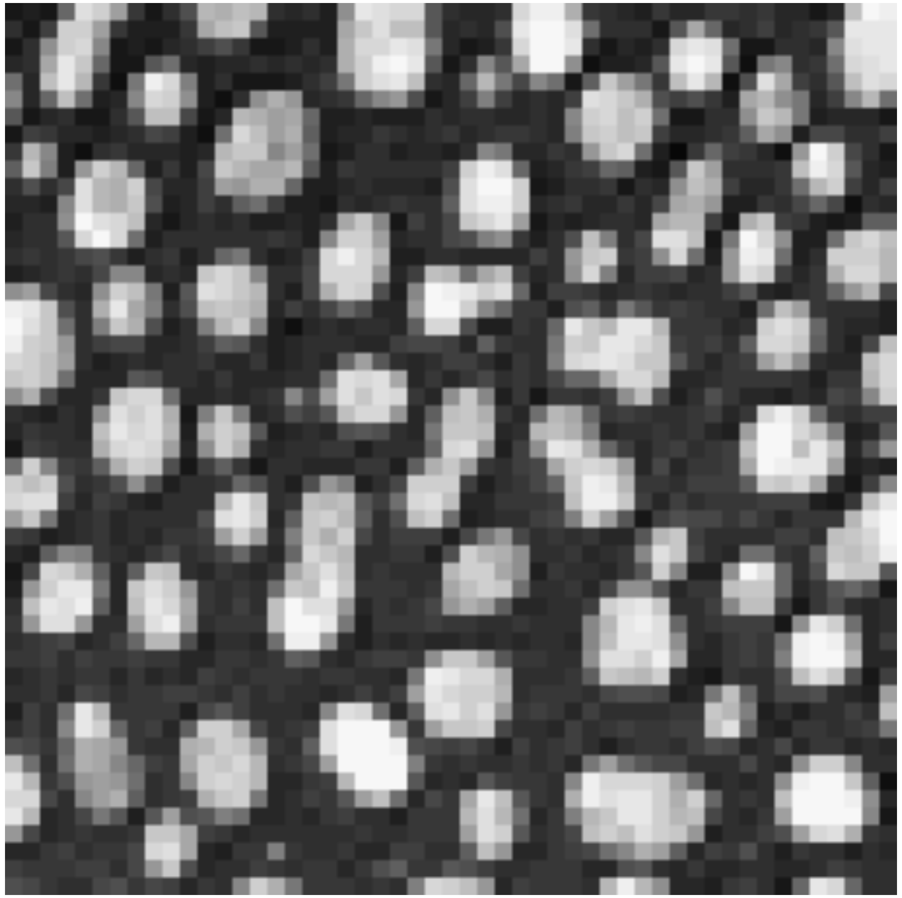
How many pixels do we need to distinguish two features in an image?



# Signal sampling



Good sampling



Not as good sampling

# Detectors in medical imaging

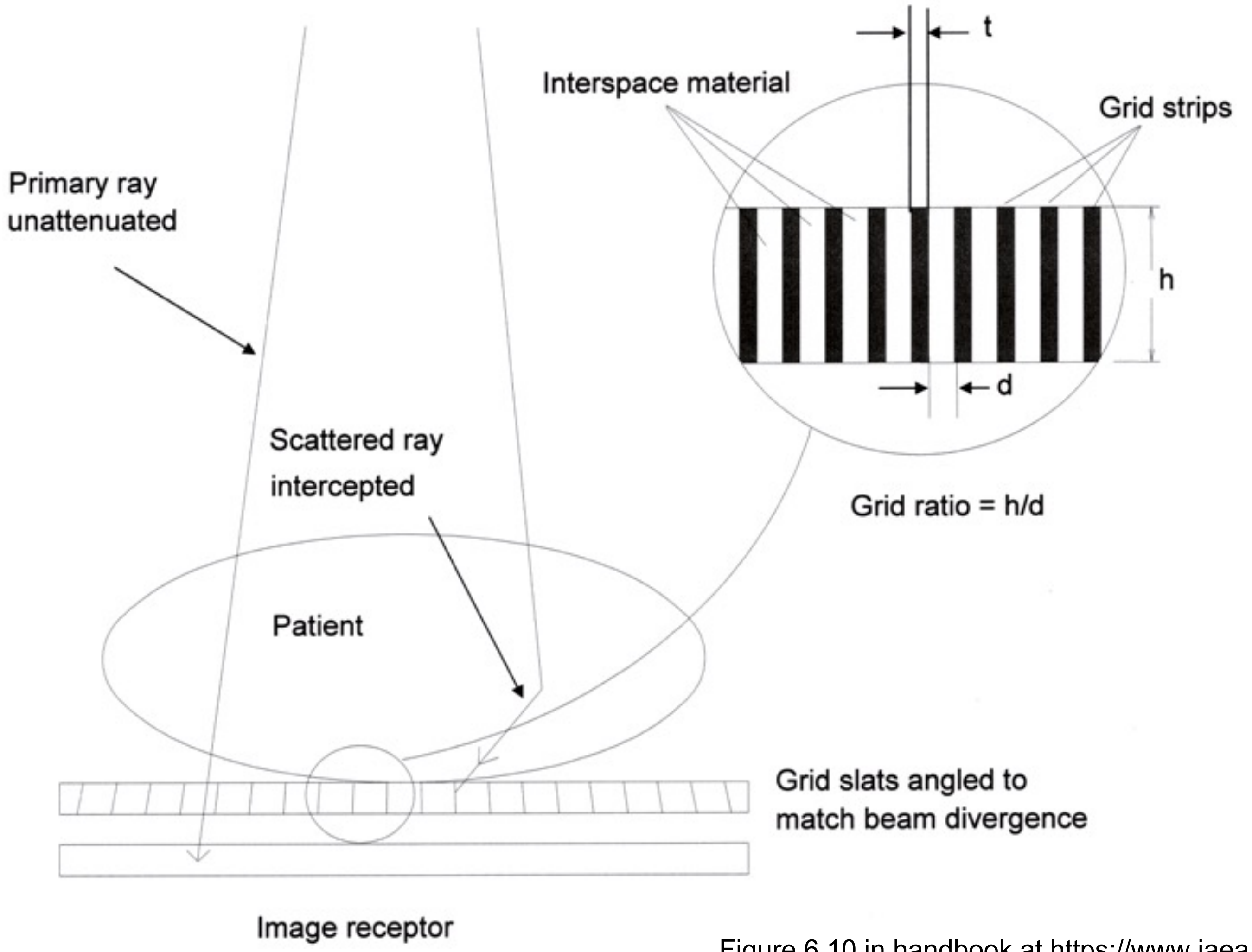



Figure 6.10 in handbook at https://www.iaea.org/publications/8841/diagnostic-radiology-physics

# X-ray safety and doses

# X-ray damage to living cells

- Directly ionizing radiation – fast charged particles such as electors
- Indirectly ionizing radiation – X-rays and gamma rays

- The physical interactions of ionizing radiation with matter lead to loss of radiation energy through ionization and the formation of free radicals.

  Direct effect of ionizing radiation

- Photons may be absorbed in the water of an organism, causing excitation and ionization in the water molecules. The radicals formed, namely the hydrated electron ($e^-$), the hydrogen atom (H·) and the hydroxyl radical (OH·), are able to diffuse far enough to reach and damage the critical targets.

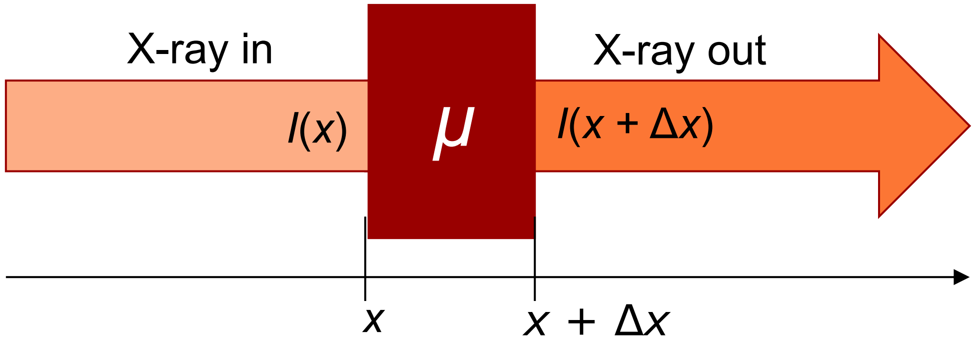
  Indirect effect of ionizing radiation

# X-ray damage to living cells

Summarized in four steps

- Ionisation
- Free radicals
- DNA damage
- Lack of cell repair

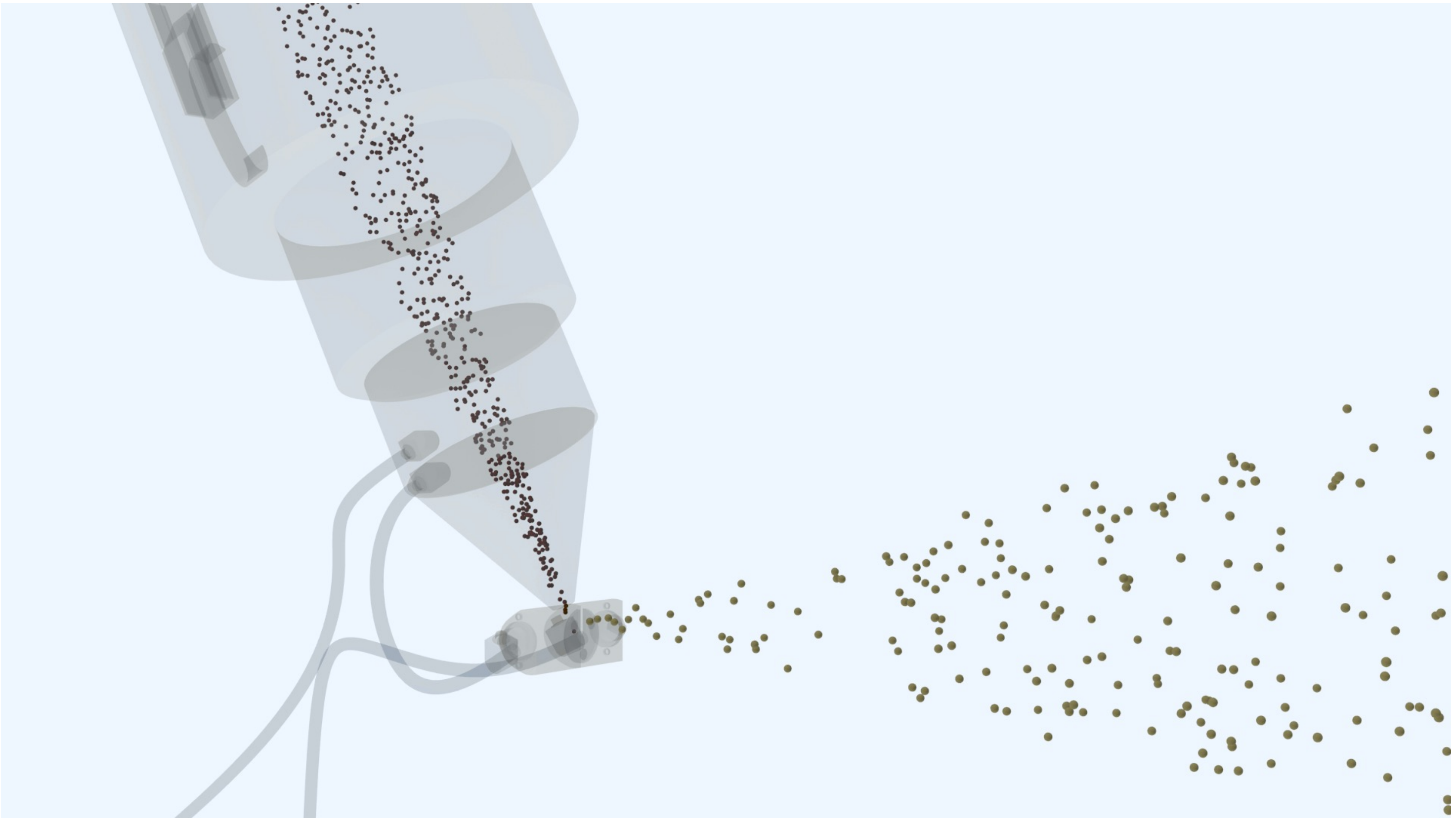
But how?




$$I(x) = I_0 e^{-\mu x}$$

# Radiation path

- How can you describe the radiation path with increasing distance from source?



Curtesy: Nikon Metrology

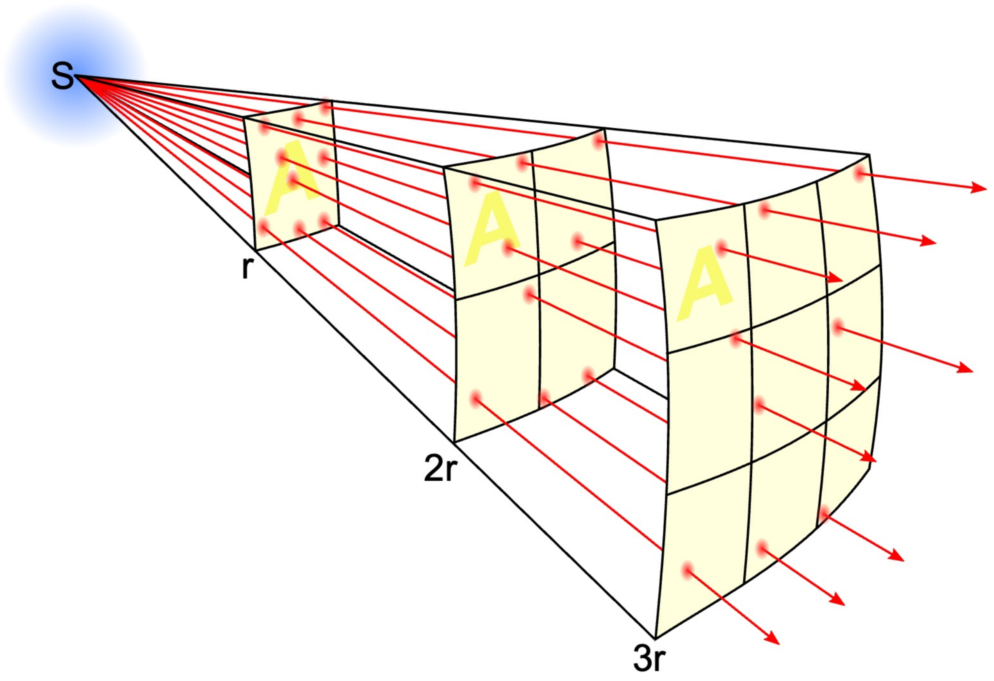
# Radiation path

- How can you describe the radiation path with increasing distance from source?

- Same description as
  - Universal law of gravity
  - Electric fields and forces
  - Intensity of light

# Radiation path

- How can you describe the radiation path with increasing distance from source?

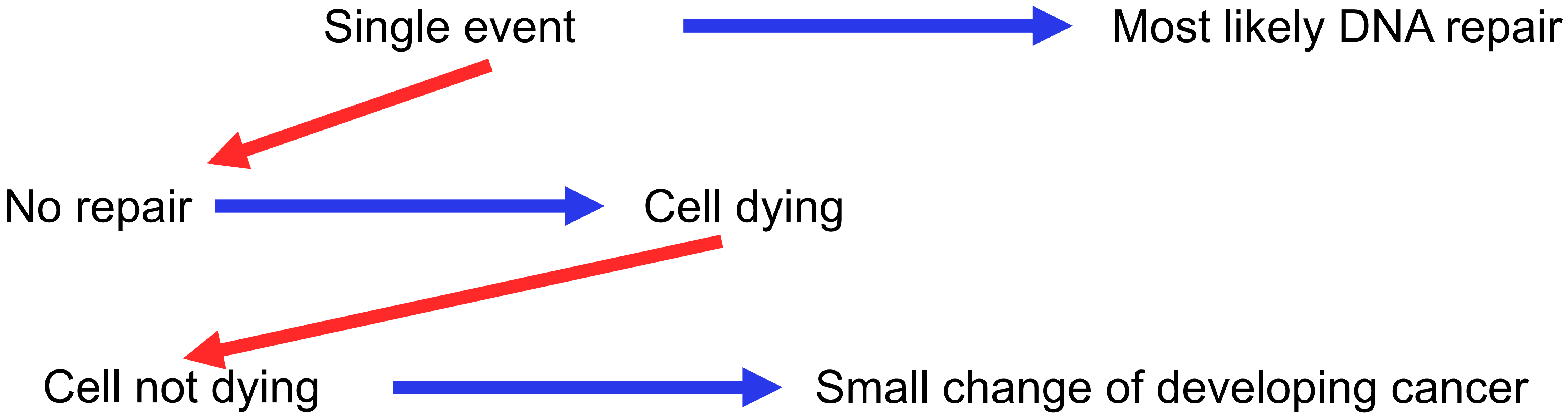



Inverse square law:

$$A \propto \frac{1}{r^2}$$

Figure from https://en.wikipedia.org/wiki/Inverse-square_law

# Back to radiation damage

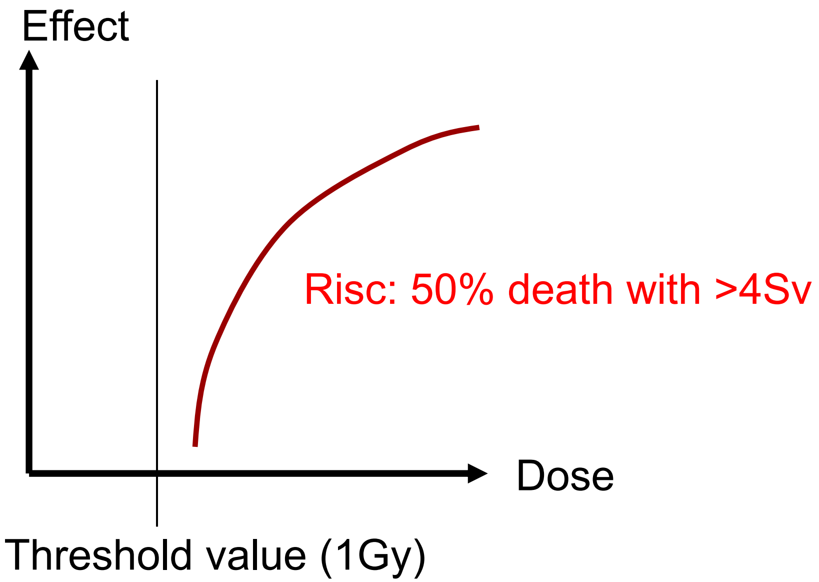



Cells under rapid cell-division are most sensitive to radiation

# Radiation damage

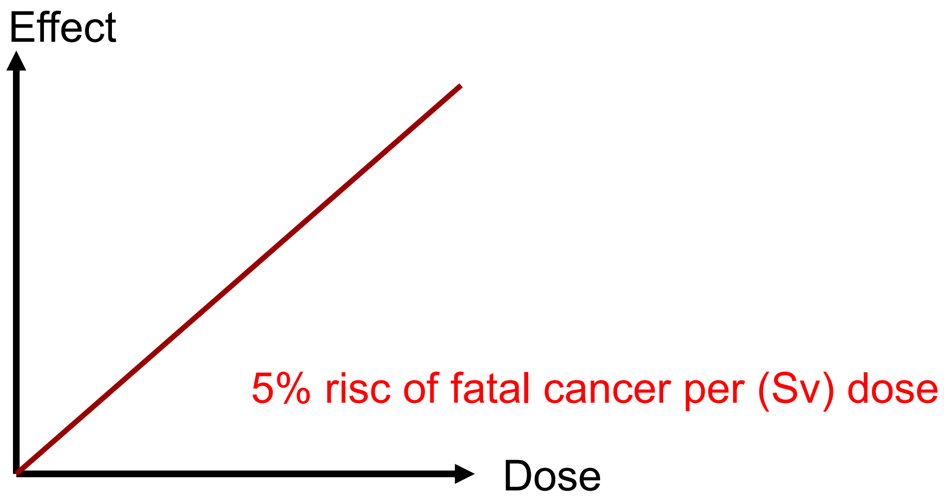
## Deterministic radiation damage

- Threshold value
- Rapid onset
- Often local damage
- Cell death




## Non-deterministic radiation damage

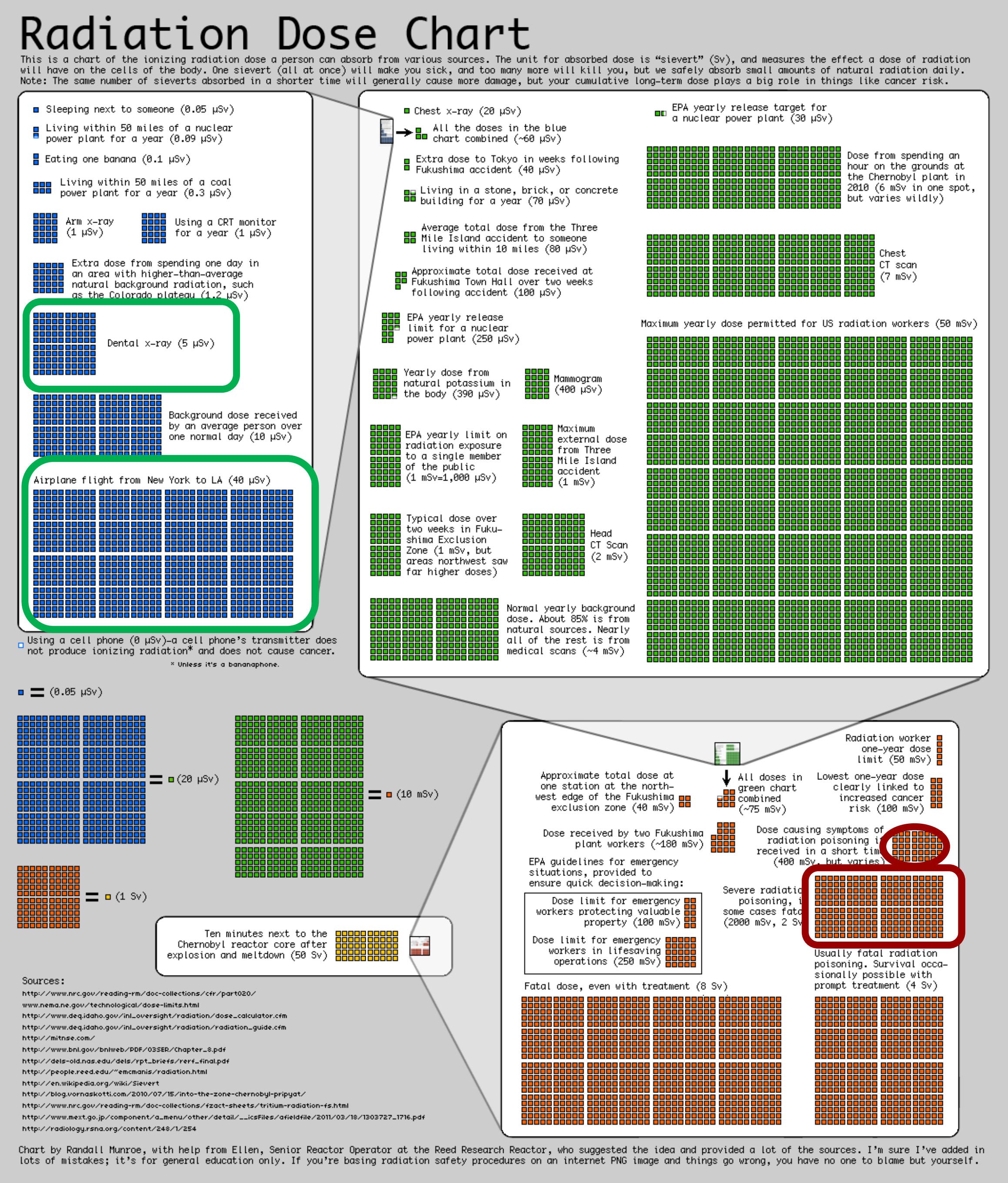
- Damage risk proportional to dose
- No known lower limit
- Damage can show up late




Se more in chapter 20 in handbook at https://www.iaea.org/publications/8841/diagnostic-radiology-physics

# Radiation dose

- Ionizing radiation
  - Unit roentgen (C/kg)
- Absorbed radiation dose
  - Gray (Gy) or rad
  - 1 Gy = 100 rad
- Different types of ionizing radiation
- Dose equivalent radiation
  - Sievert (Sv)
  - 1 Sv = 100 rem




https://www.convert-me.com/en/convert/radiation/

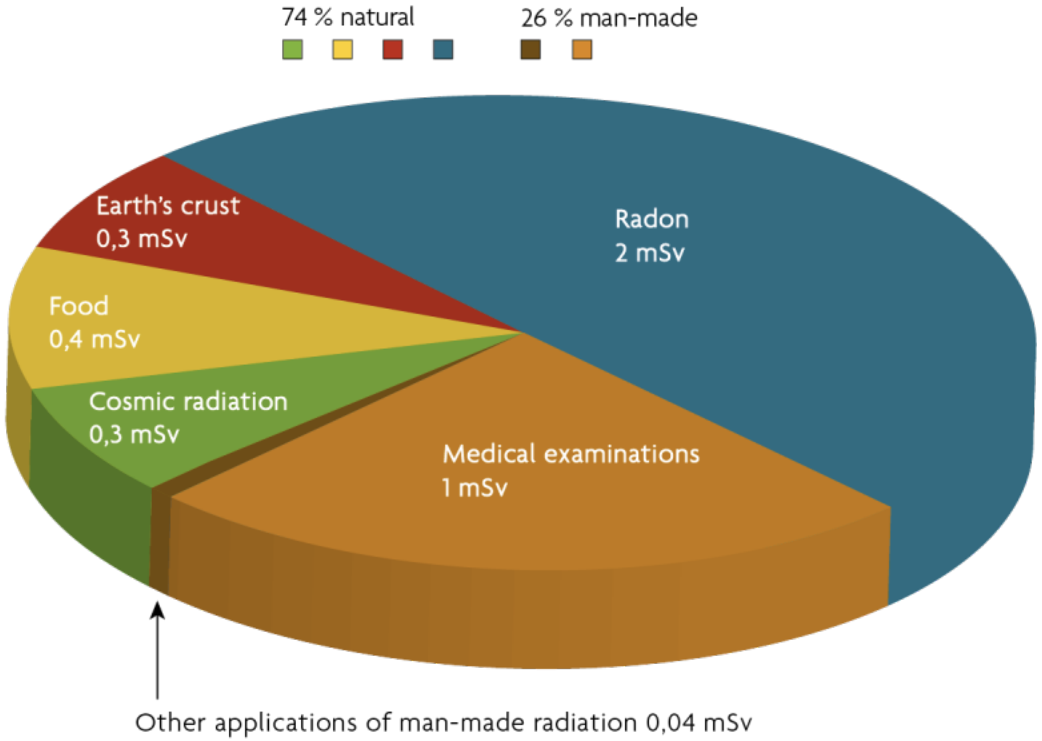
# Radiation dose in medical examinations

Table 2. Comparison of typical doses in UK from CT and conventional x-ray examinations (RCR, 1998)

| Diagnostic procedure | Typical effective dose (mSv) |
|---|---|
| *Conventional x-ray procedure* | |
| Limbs and joints | $<0.01$ |
| Chest (single PA film) | 0.02 |
| Skull | 0.07 |
| Thoracic spine | 0.7 |
| Lumbar spine | 1.3 |
| Hip | 0.3 |
| Pelvis | 0.7 |
| Abdomen | 1.0 |
| IVU | 2.5 |
| Barium swallow | 1.5 |
| Barium meal | 3 |
| Barium follow through | 3 |
| Barium enema | 7 |

# How much radiation for average person

Residents in Denmark receive in average 4 mSv per year




[Document from Danish Health Authority - Radiation Protection]

3D Imaging Center at DTU