Instrumental Technique Presentation

X-ray source

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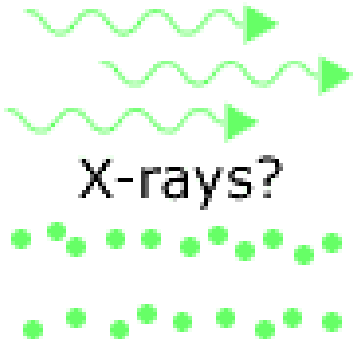
6.08.18

X-rays, What Are They?

- In 1895, Wilhelm Rontgen, a German physicist discovered X-rays
- They are electromagnetic waves of shorter wavelength and higher energy than normal light.



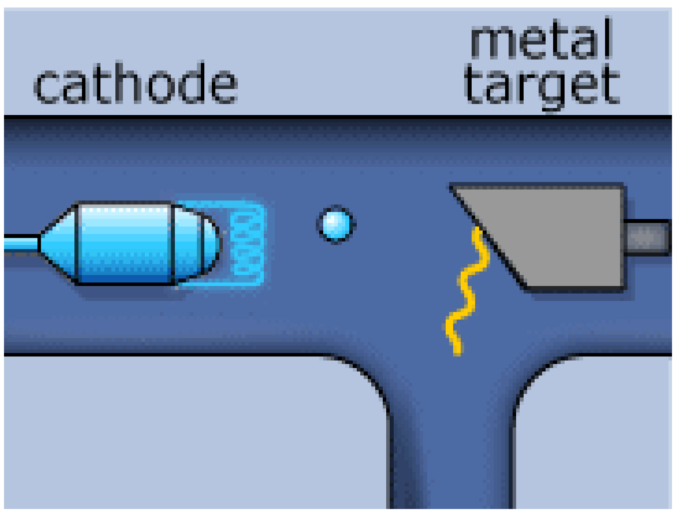
The nature of the rays – waves or particles?

In 1920, wave-particle duality was accepted and according to this theory photons can be described both as waves and particles.

How Are X-rays Made?

- To generate X-rays, three things are needed

1. a source of electrons
2. a means of accelerating the electrons at high speeds
3. a target material to receive the impact of the electron to interact with them



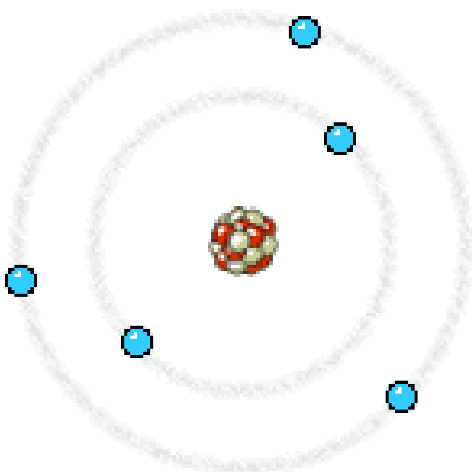
X-rays are produced when electrons strike a metal target. The electrons are liberated from the heated filament and accelerated by a high voltage towards the metal target. The X-rays are produced when the electrons collide with the atoms and nuclei of the metal target.

- The maximum energy of the produced X-ray photon is limited by the energy of the incident electron, which is equal to the voltage on the tube times the electron charge ($E = eV$), so an 80 kV tube cannot create X-rays with an energy greater than 80 keV.

- When the electrons hit the target, X-rays are created by two different atomic processes:

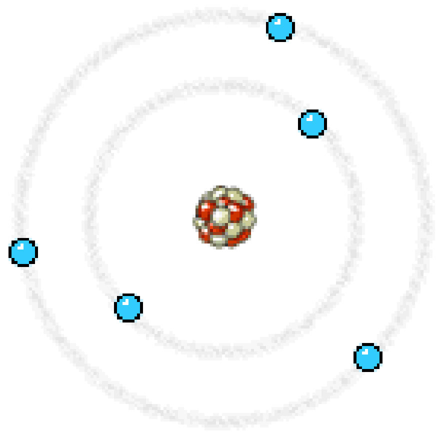
1. Bremsstrahlung X-rays
2. Characteristic X-rays

Bremsstrahlung X-rays



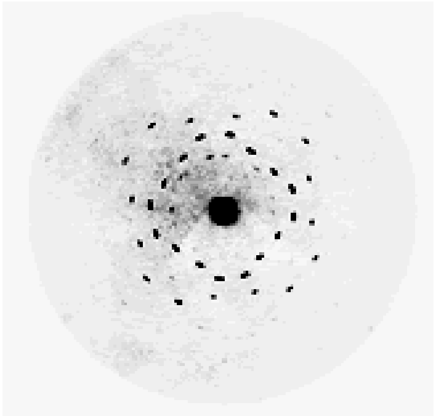
In an X-ray tube the electrons emitted from the cathode are accelerated towards the metal target anode by an accelerating voltage of typically 50 kV. The high energy electrons interact with the atoms in the metal target. Sometimes the electron comes very close to a nucleus in the target and is deviated by the electromagnetic interaction. In this process, which is called bremsstrahlung (braking radiation), the electron loses much energy and a photon (X-ray) is emitted. The energy of the emitted photon can take any value up to a maximum corresponding to the energy of the incident electron.

Characteristic X-ray



The high energy electron can also cause an electron close to the nucleus in a metal atom to be knocked out from its place. This vacancy is filled by an electron further out from the nucleus. The well defined difference in binding energy, characteristic of the material, is emitted as a monoenergetic photon. When detected this X-ray photon gives rise to a characteristic X-ray line in the energy spectrum. C. Barkla observed these lines in 1908-09 and was given the 1917 Nobel Prize for this discovery. He also made the first experiments suggesting that the X-rays are electromagnetic waves.

X-rays Behave Like Light!



Interference pattern observed by von Laue and collaborators using a photographic plate. The large central spot is due to the unscattered X-ray beam. The dark spots correspond to directions where X-rays scattered from different crystal (ZnS) layers interfere constructively.

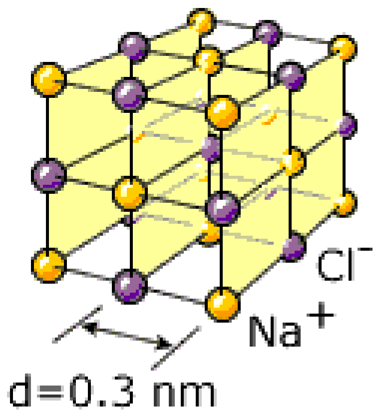
X-rays Reveal Crystal Structures

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

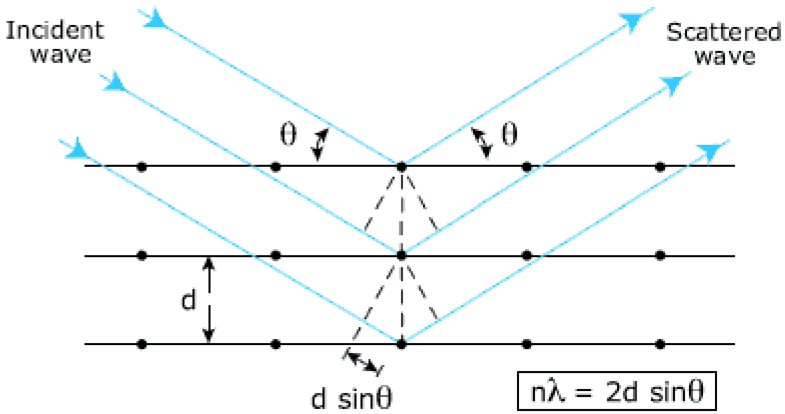
William Henry Bragg and his son William Lawrence developed the method to analyze crystal structures using X-rays.

The famous Bragg formula relates the wavelength λ of the X-ray with the distance d between crystal planes and the incident angle of the X-ray Θ giving rise to constructive interference.

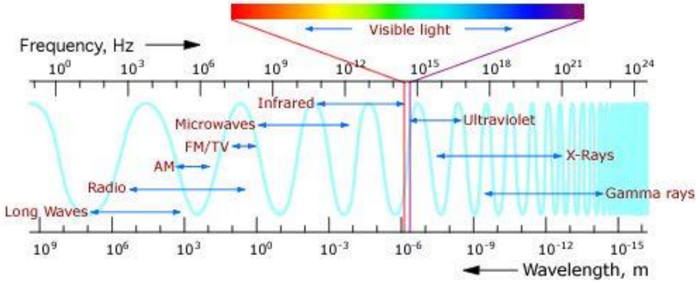
For their analysis of crystal structures they were awarded the 1915 Nobel Prize.



Crystal planes in NaCl



X-rays have wavelengths much shorter than visible light, but longer than high energy gamma rays. Their wavelength is well suited to study crystal structures and details of the human body. In addition, several objects and processes in the Universe emit X-rays. These X-rays are the messangers revealing information of the cosmos.



Types of X-ray sources

X-ray sources can be classified into three types:

1. X-ray tube
   a. Sealed X-ray tube
   b. Rotating anode tube
   c. Microfocus X-ray tube
2. Synchrotron radiation
3. Free electron laser

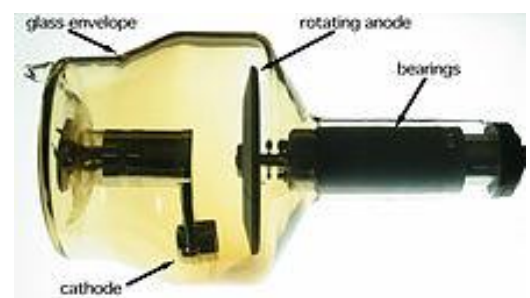
1) Typical cathode element W
2) Potential difference 20-50 kV
3) Anode must be water cooled
4) Frequency depends on the anode materials, Cu, Mo, Co etc.

➢ Sealed X-ray tube

The simplest and cheapest variety of sealed X-ray tube has a stationary anode (the Crookes tube) and run with ~2 kW of electron beam power. Tungsten is used as cathode and copper is used as anode.

➢ Rotating anode

The anode is supported on vacuum bearings and can be rotated by electromagnetic induction from a series of stator windings outside the evacuated tube. The anode must be constructed of high temperature materials. Typical materials are a tungsten-rhenium target on a molybdenum core, backed with graphite. It run with ~14 kW of e-beam power.



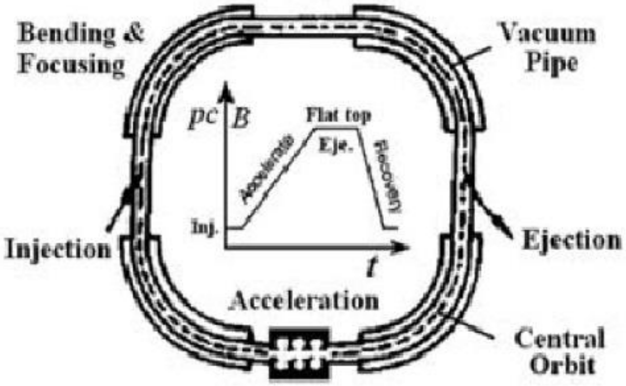
➢ Microfocus X-ray tube

- ✓ Some X-ray examinations (such as, e.g., non-destructive testing and 3-D microtomography) need very high-resolution images and therefore require X-ray tubes that can generate very small focal spot sizes, typically below 50 µm in diameter. These tubes are called microfocus X-ray tubes.

- ✓ There are two basic types of microfocus X-ray tubes:
  - a. solid-anode tubes
  - b. metal-jet-anode tubes.

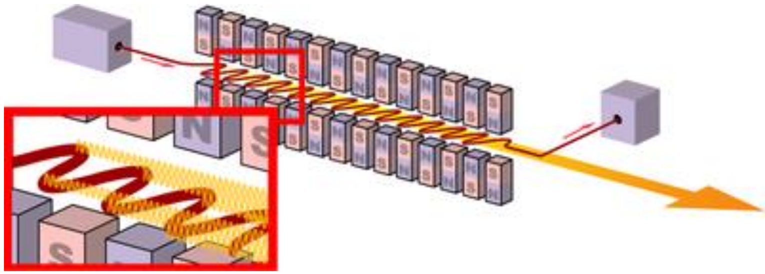
➢ Synchrotron radiation

It is the single most powerful tool available to X-ray crystallographers. It is made of X-ray beams generated in large machines called synchrotrons. These machines accelerate electrically charged particles, often electrons, to nearly the speed of light and confine them in a (roughly) circular loop using magnetic fields.



➢ Free electron laser

These are the brightest X-ray sources currently available; with the X-rays coming in femtosecond bursts. The intensity of the source is such that atomic resolution diffraction patterns can be resolved for crystals otherwise too small for collection.



Brilliance

When comparing X-ray sources, an important measure of quality of the source is called *brilliance*. Brilliance takes into account:

1. Number of photons produced per second
2. The angular divergence of the photons, or how fast the beam spreads out
3. The cross-sectional area of the beam
4. The photons falling within a bandwidth (BW) of 0.1% of the central wavelength or frequency

The resulting formula is:

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

The greater the brilliance, the more photons of a given wavelength and direction are concentrated on a spot per unit of time.

Cu-Mo dual source used in single crystal XRD


Thank you!