PHYSICS OF CRYSTALS

Chapter 1

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INTRODUCTION

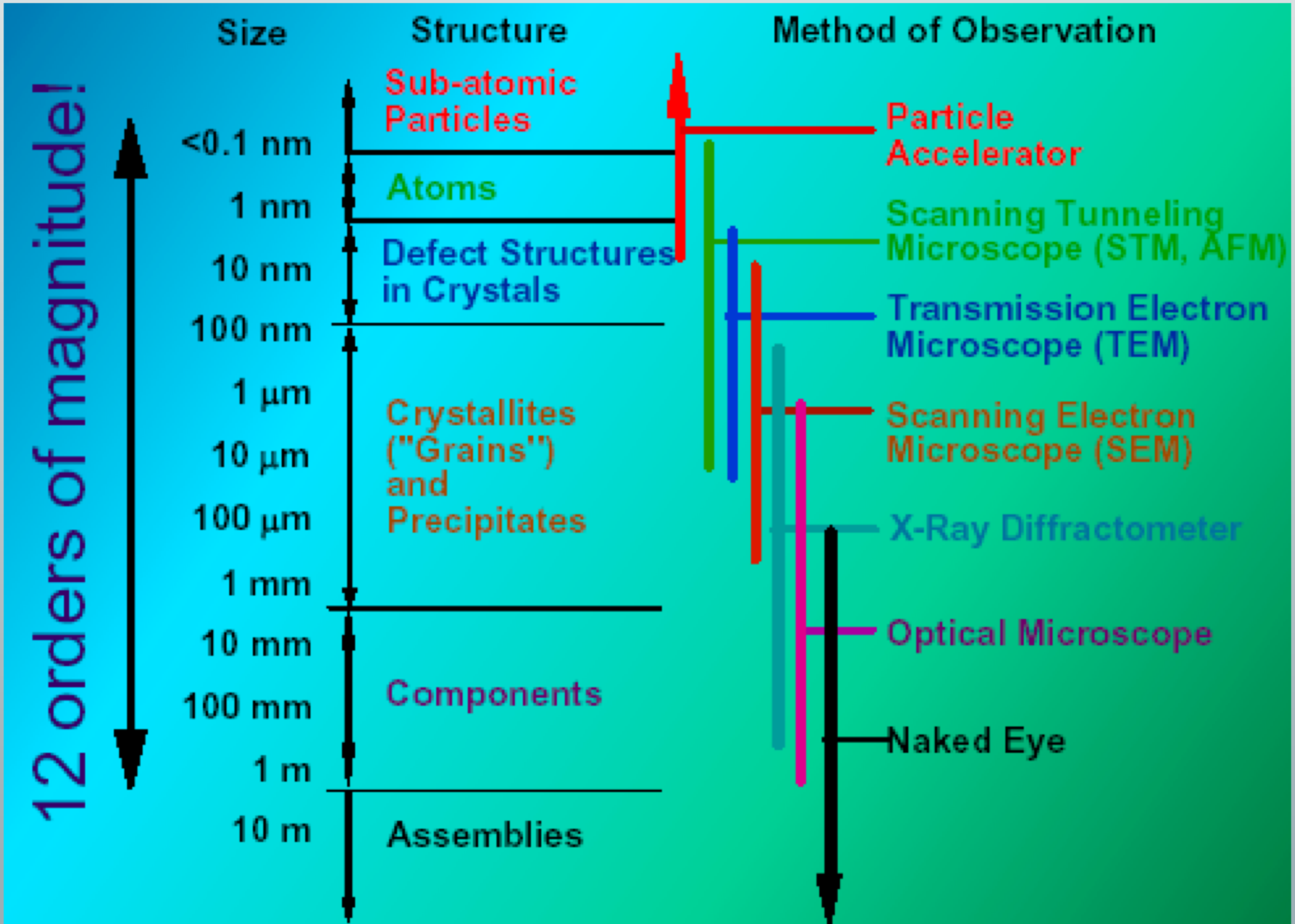
- **X-ray crystallography is a method used to study the atomic and molecular structure of a crystal and is based on the diffraction of the rays in an X-ray beam of crystalline atoms in various directions specific to the crystal. By measuring the angles and amplitudes of these diffracted beams, a crystallographer can obtain a three-dimensional image of the density of electrons in the crystal. From this electron density, the average positions of the atoms in the crystal can be determined along with chemical bonds, irregularities in the crystal structure and some other information.**
- Since salts, metals, minerals, semiconductors as well as various inorganic, organic and biological molecules can form crystals, X-ray crystallography has been the basis for many scientific fields. Since its discovery, this method has been used to find the size of the atoms of various materials, especially minerals and alloys, the length and types of chemical bonds, and atomic scale differences..

INTRODUCTION

- The method revealed the structure and function of many biological molecules, including vitamins, drugs, proteins and nucleic acids such as DNA. X-ray crystallography is still the main method used to describe the atomic structure in new materials and to understand the similarities between materials subject to different experiments. The crystal structures understood by X-ray can explain the unconventional new electronic and flexibility properties of a material, shed light on a chemical interaction process, or serve as the basis for the design of new drug substances against disease.

INTRODUCTION

- When the crystal is placed on a protractor in an X-ray diffraction measurement, it is bombarded with X-rays as it is slowly rotated, resulting in a pattern of regularly spaced spots known as reflections. The two-dimensional images obtained from different angles are combined with the known chemical data of the sample using the mathematical Fourier transform method, and a three-dimensional model of the electrons in the crystal is obtained.

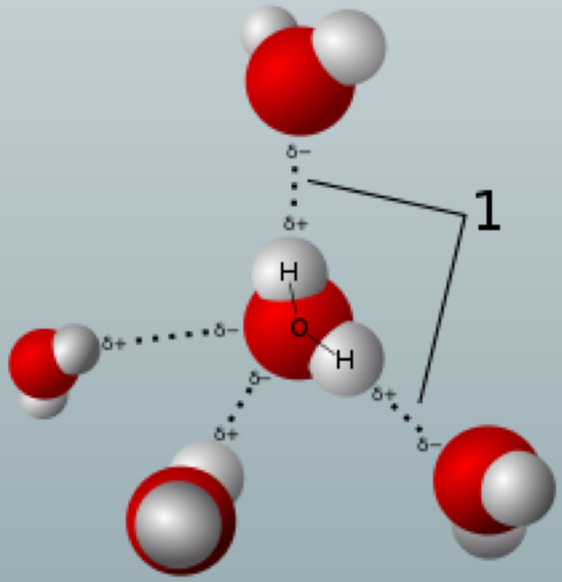


HISTORY

- Crystals have long attracted attention because of their order and symmetry, but were not studied scientifically until the 17th century. In a study by Johannes Kepler Strena seu de Nive Sexangula (1611), he hypothesized that the hexagonal symmetries of snowflakes are due to the regular arrangement of spherical water particles.
- Crystal symmetry was experimentally demonstrated by Nicolas Steno (1669), a Danish scientist who was the first to prove that the angles between all faces of a given crystal in any sample are always the same, and that each face of a crystal is stacked as simple blocks of the same size and shape. It was explored by René Just Haüy (1784) who discovered that it could be identified.

HISTORY

- Thus, in 1839, William Hallowes was able to give three small integer labels to each hundred. Today Miller indices are still used to describe the faces of crystals. Haüy's work thought that the crystals were in the form of regular three-dimensional arrays of atoms and molecules (a Bravais lattice), and that the unit cell repeats continuously along three fundamental axes that are not necessarily perpendicular to each other.
- A complete catalog of possible symmetries in the 19th century was put forward by Johan Hessel, Auguste Bravais, Evgraf Fedorov, Arthur Schönflies and William Barlow. From available data and physical explanations, Barlow proposed many crystal structures in the 1880s that were later validated by X-ray crystallography; however, the model was not found convincing because the available data in the 1880s were very inadequate.



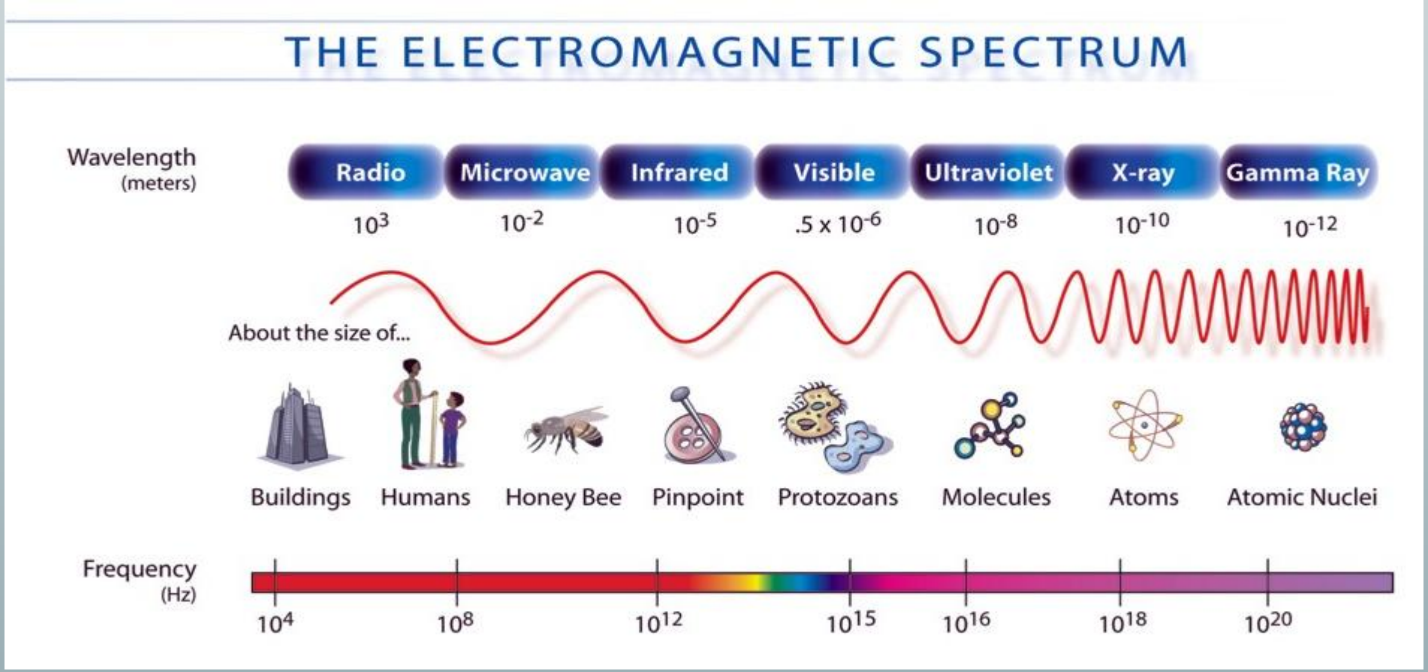
HISTORY

- X-rays were discovered by Wilhelm Conrad Röntgen in 1895, when theoretical studies on crystal symmetry were concluded. Physicists initially did not know exactly the nature of X-rays (although they had accurate predictions that it is an electromagnetic radiant wave, that is, a different form of light). At that time, the wave model of light — especially Maxwell's theory of electromagnetic radiation — was well accepted in scientific circles.
- Single slit experiments in Arnold Sommerfeld's lab showed that the wavelengths of X-rays were around 1 angstrom. However, since X-rays consisted of photons, it also showed a grain feature. The concept of photon was introduced by Albert Einstein in 1905, but was not widely accepted until 1922, when it was confirmed by Arthur Compton with the scattering experiment of X-rays from electrons.
- Hence, the particle properties of X-rays, such as ionizing gases, led William Henry Bragg to make claims in 1907 that X-rays were not electromagnetic waves. However, Bragg's point of view was not well accepted and as a result of the observation of X-ray diffraction in 1912, it was accepted by most scientists that X-rays were a kind of electromagnetic radiation.

HISTORY

X-rays are electromagnetic waves or photon beams with an energy range of 0.125 to 125 keV or corresponding wavelengths in the range of 10 to 0.01 nm. It is equivalent to the range of vibration numbers in the range of 30 to 30,000 PHz (1015 hertz).

- X-rays are used especially for diagnostic purposes in medicine. Since they belong to the ionizing radiation class, they can be harmful. X-rays were discovered in 1895 as a result of experiments by Wilhelm Conrad Röntgen. Within the boundaries of classical physics, X-rays are electromagnetic waves just like visible light, and their difference from visible light is their low wavelength, hence their high frequency and energy. It is beyond ultraviolet. Beyond the X-Rays are Gamma rays.



HISTORY

- X-rays are also called X-rays. The term X-ray (German: X Strahlung, today Röntgenstrahlung) was first discovered by Wilhelm Conrad Röntgen, who discovered these rays but could not find their exact properties, and used it to mean "unknown". It is now known that X-rays are part of the electromagnetic radiation spectrum. These rays have wavelengths between 10−9 and 10−11cm. Wavelength is shorter than that of visible light.

Anna Bertha Röntgen

In 1895 Röntgen discovers X-rays

Wilhelm Röntgen

1901: The First Nobel Prize in Physics
Wilhelm Conrad Röntgen

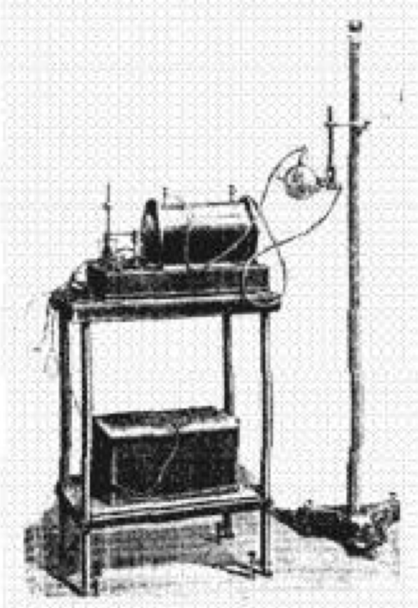
Prize motivation: "in recognition of the extraordinary services he has rendered by the discovery of the remarkable rays subsequently named after him"

X-RAYS

- X-rays, which form the basis of today's imaging methods and opened a new era in medical science, were discovered in 1895 by German Physics Professor Wilhelm Conrad Röntgen.
- Röntgen, who moved to the University of Würzburg, found the X-rays while working at this University on 8 November 1895. X-ray at that time; By connecting a Crooks tube to an induction coil, he observed that when a high-voltage electric current was passed through the tube, some sparkles were formed in the barium platinum crystals in a glass jar that was located quite far from the tube; He named the rays that cause such glitters "X-rays" because they were unknown until then.

- Röntgen observed that when high voltage current was passed through the tube, the rays that create glows on the screen opposite could pass different objects at different degrees, and they were captured by lead plates, and while examining the shadow of the lead plates he held with his hand, he also noticed the shadows of his own finger bones.

- Upon this incident, he obtained the image of his finger bones and ring by placing his wife's hand on a tape containing a photographic record. X-ray, first presented its determinations and the images obtained by this method on December 28, 1895 at the Würtzburg Physical Medicine Society, and with this invention, the first simple x-ray devices began to be manufactured.
- W. C. Röntgen, who was awarded the Nobel Prize in Physics for the first time in 1901, died in 1923 at the age of 78. While Röntgen's discovery of X-rays had great repercussions in the scientific community, it also led to new developments. Shortly after this discovery, H. Antonie Becquerel studied the radioactivity of uranium while working on X-rays; Curies, on the other hand, discovered the radium element and realized the birth of a new science called "Radiology".



- 1896 Yılında kullanılan İlk Röntgen cihazlarından bir. (Sağ üstte)
- X – Işını Tüpü (Sol üstte).
- İlk Görüntüleme Örneği (Sol altta).

- X-rays are electromagnetic waves with wavelengths varying between 0.1-100 Å, which are caused by the slowing of high-energy electrons or by electron transitions in the inner orbits of atoms.
- X-rays with small wavelengths and high degrees of penetration are called "hard X-rays", X-rays with large wavelengths and low penetration degrees are called "soft X-rays".
- X-rays with wavelengths of 0.5-2.5 Å (soft) in crystallography and 0.5-1 Å (hard) in radiology are used. The frequency of X-rays is, on average, 1000 times greater than the frequency of green light, and the X-ray photon (particle) has higher energy than the photon of the visible light.
- Therefore, the two characteristics that determine these rays are their short wavelength and high energy.
- X-rays show both wave and particle properties. Therefore, they have double characters. Photoelectric absorption, Compton scattering (incoherent scattering), gas ionization and scintillation particle properties; velocity, polarization and Rayleigh scattering (coherent scattering) are wave properties. Electromagnetic radiation showing particle character is called photon.

Çizelge: X-ışınlarının Genel Özellikleri ve Madde Etkileşmesi

Genel Özellikler	Etkileşme sonucu maddeden çıkan tanecik
• Sürekli spektrum verir. • Çizgi spektrum verir. • Işık hızı ile yayılır. • Doğrular halinde yayılır. • Elektrik ve magnetik alandan etkilenmezler.	• İyon • Fotoelektron • Auger elektronu • Geri tepme elektronu • Elektron pozitron çifti
Yapabileceği fiziksel olaylar	**X-ışını soğurmasının kalıcı sonuçları**
• Transmisyon • Kırılma • Yansıma • Polarizasyon • Koherent saçılma • İnkoherent saçılma • Fotoelektrik olay	• Radyasyon tahribatı • Sıcaklık artması • Fotoelektrik iyonizasyon • Genetik değişme • Hücrenin ölümü

Elektromanyetik spektrumda gama ışınları ile mor ötesi ışınlar arasında yer alırlar.