TEJASVI NAVADHITAMASTU

"Let our (the teacher and the taught) learning be radiant"

Let our efforts at learning be luminous and filled with joy, and endowed with the force of purpose

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E –content

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Topic: Instrumentation and Analytical Techniques
Subtopic: **X-Ray Diffraction**
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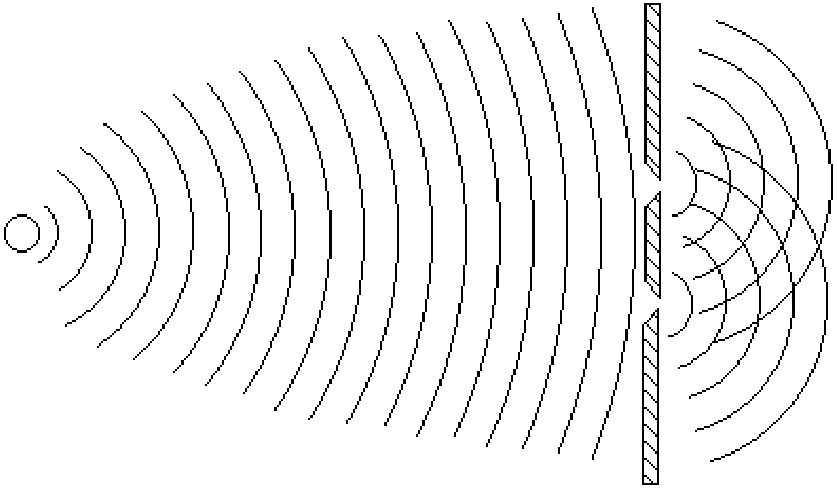
X-Ray Diffraction

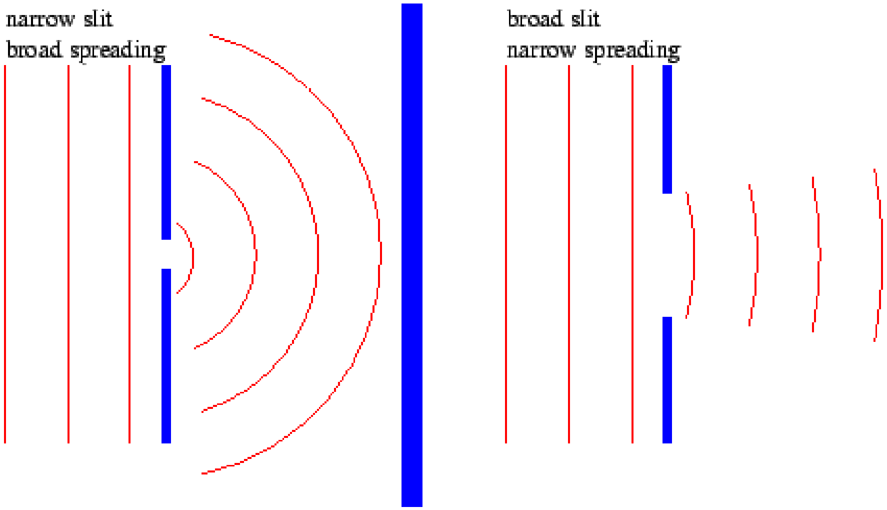
X Ray: An electromagnetic wave of high energy and very short wavelength (between ultraviolet light and gamma rays), which is able to pass through many materials opaque to light.

Energy : 100 eV to 100keV
Wavelength : 0.01 to 10 nanometer

Diffraction

The process by which a beam of light or other system of waves is spread out as a result of passing through a narrow aperture or across an edge, typically accompanied by interference between the wave forms produced.





X Ray Diffraction

- A technique used to determine the atomic and molecular structure of a crystal, in which the crystalline atoms cause a beam of incident X-rays to diffract into many specific directions.

- The atomic planes of a crystal cause an incident beam of X-rays to interfere with one another as they leave the crystal. The phenomenon is called X-ray diffraction.

- A stream of X-rays directed at a crystal diffract and scatter as they encounter atoms. The scattered rays interfere with each other and produce spots of different intensities that can be recorded on film.

- X-ray crystallography is a tool used for identifying the atomic and molecular structure of a crystal, in which the crystalline atoms cause a beam of incident X-rays to diffract into many specific directions. By measuring the angles and intensities of these diffracted beams, acrystallographer can produce a three-dimensional picture of the density of electrons within the crystal. From this electron density, the mean positions of the atoms in the crystal can be determined, as well as their chemical bonds, their disorder and various other information.

Principles

The interaction of electromagnetic radiation with matter causes the electrons in the exposed sample to oscillate. The accelerated electrons, in turn, will emit radiation of the same frequency as the incident radiation, called the secondary waves. The superposition of waves gives rise to the phenomenon of interference.

Depending on the displacement (phase difference) between two waves, their amplitudes either reinforce or cancel each other out. The maximum reinforcement is called constructive interference, the cancelling is called destructive interference. The interference gives rise to dark and bright rings, lines or spots, depending on the geometry of the object causing the diffraction.

Diffraction effects increase as the physical dimension of the diffracting object (aperture) approaches the wavelength of the radiation. When the aperture has a periodic structure, for example in a diffraction grating, repetitive layers or crystal lattices, the features generally become sharper.

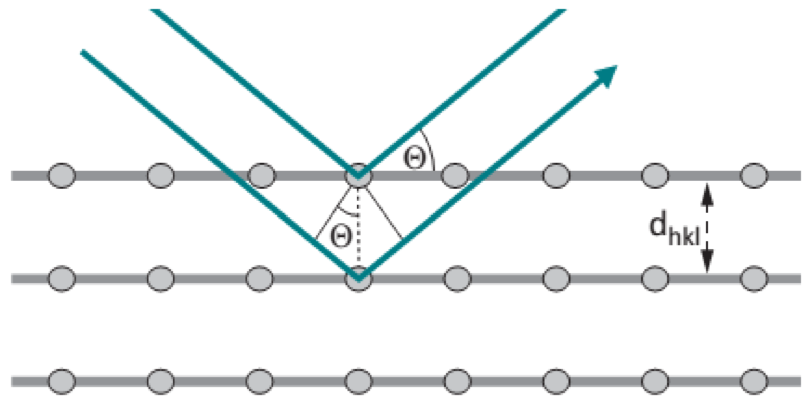
Bragg’s law describes the condition that waves of a certain wavelength will constructively interfere upon partial reflection between surfaces that produce a path difference only when that path difference is equal to an integral number of wavelengths. From the constructive interferences, i.e. diffraction spots or rings, one can determine dimensions in solid materials.

Bragg's Law

Bragg's law was used to explain the interference pattern of X-rays scattered by crystals

Two beams with identical wavelength and phase approach a crystalline solid and are scattered off two different atoms within it. The lower beam traverses an extra length of $2d\sin\vartheta$. Constructive interference occurs when this length is equal to an integer multiple of the wavelength of the radiation.

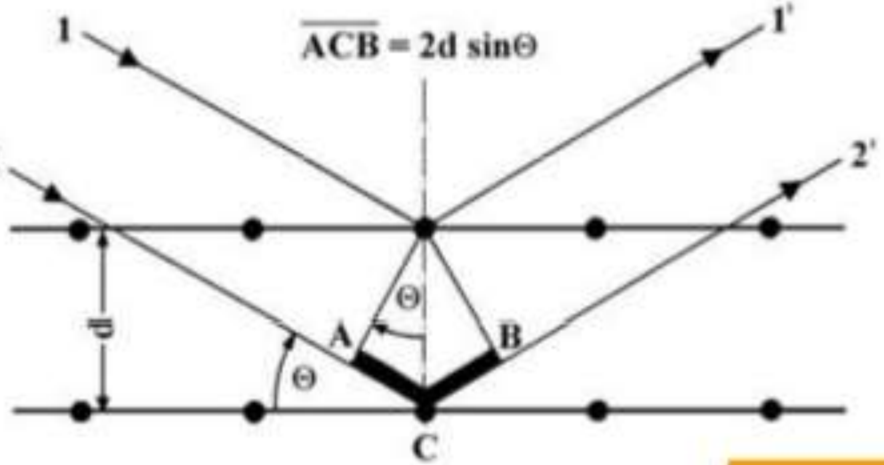
$$N\lambda = 2_{dhkl} \sin\theta$$



Bragg's law. Interference effects are observable only when radiation interacts with physical dimensions that are approximately the same size as the wavelength of the radiation. Only diffracted beams that satisfy the Bragg condition are observable (constructive interference). Diffraction can thus be treated as selective reflection. n is an integer ('order'), λ is the wavelength of the radiation, d is the spacing between the lattice planes and Θ is the angle between the incident/reflected beam and the lattice plane.

BRAGG'S LAW OF DIFFRACTION

No peak is observed unless the condition for constructive interference ($\delta = n\lambda$, with n an integer) is precisely met:



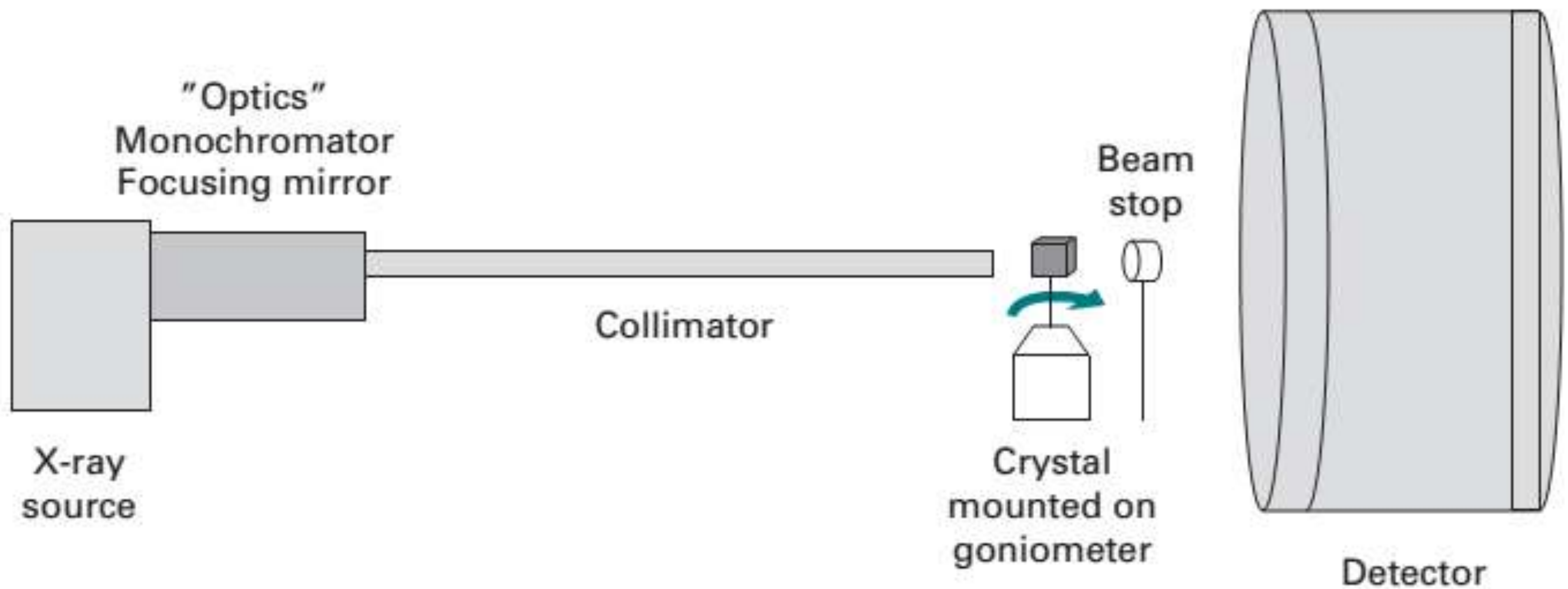
$$\overline{AC} = d \sin\theta$$

$$\overline{ACB} = 2d \sin\theta$$

$$n\lambda = \overline{ACB}$$

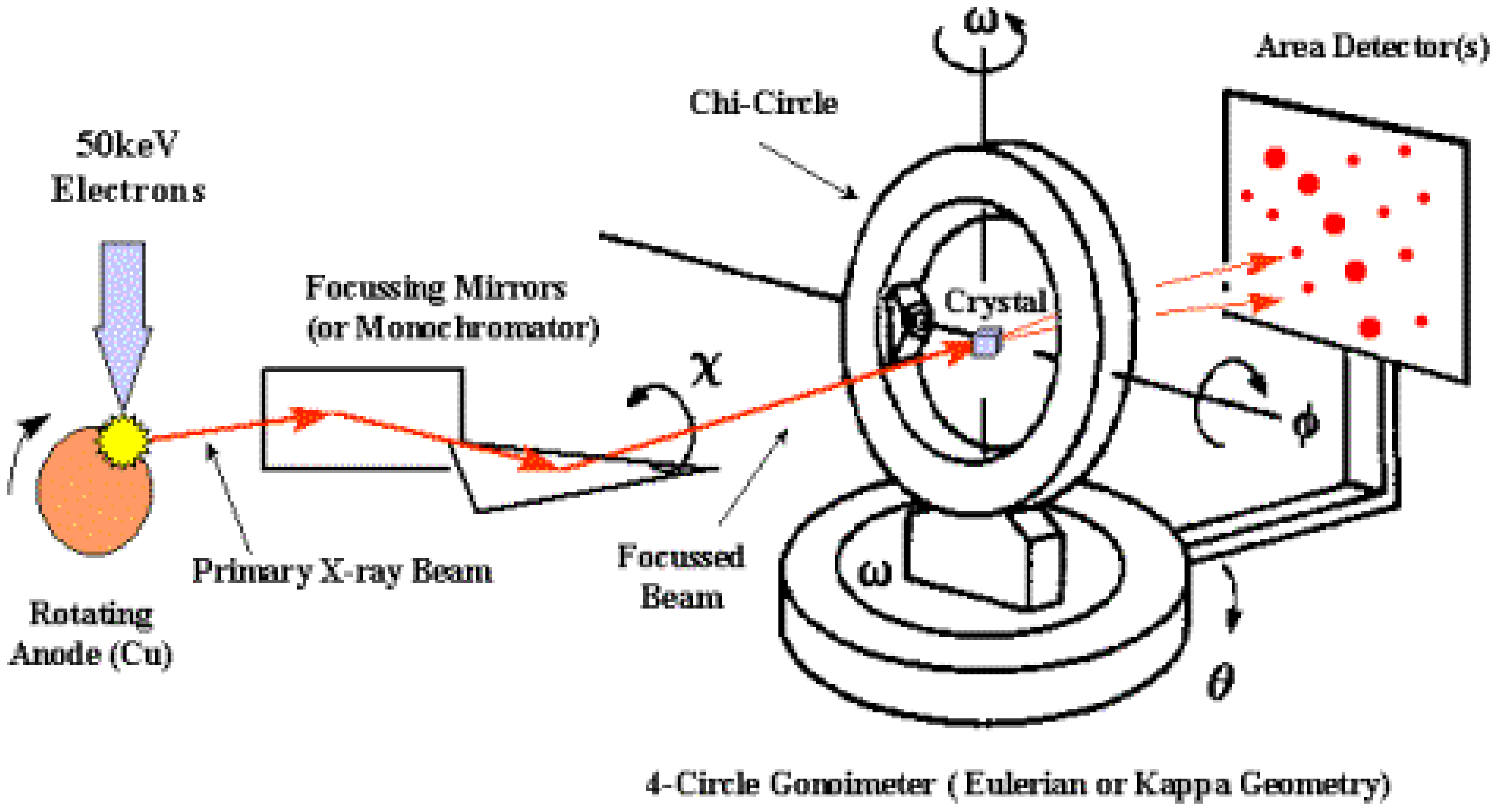
Bragg's Law: $n\lambda = 2d \sin\theta$

When Bragg's Law is satisfied, "reflected" beams are in phase and interfere constructively. Specular "reflections" can occur only at these angles.

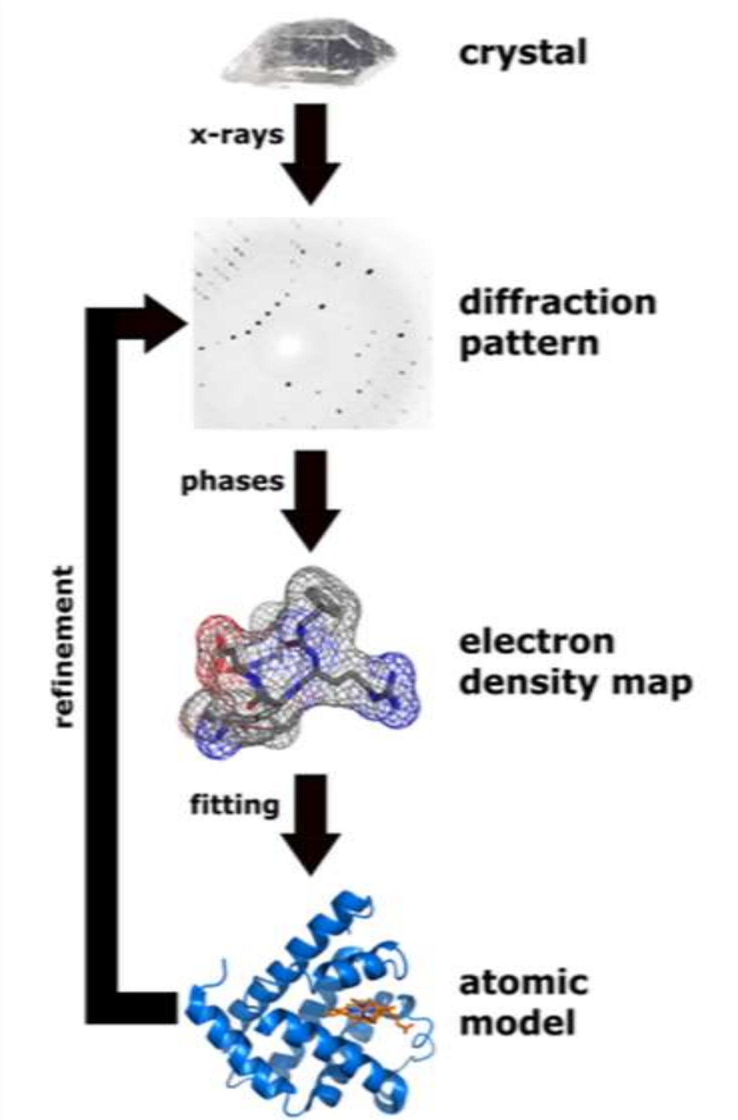


Instrumentation for X-ray diffraction. The most common X-ray sources are (a) particle storage rings which produce synchrotron radiation, and (b) rotating anode tubes. The schematics of an X-ray diffractometer are shown in (c).

Experimental Setup



How Does It Work



Crystal (regular array of atoms) is mounted on a Goniometer

↓

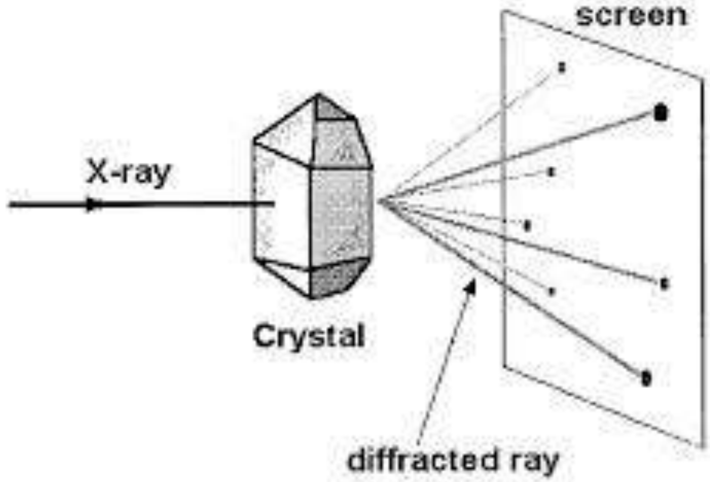
Bombarded with X-Ray while rotating

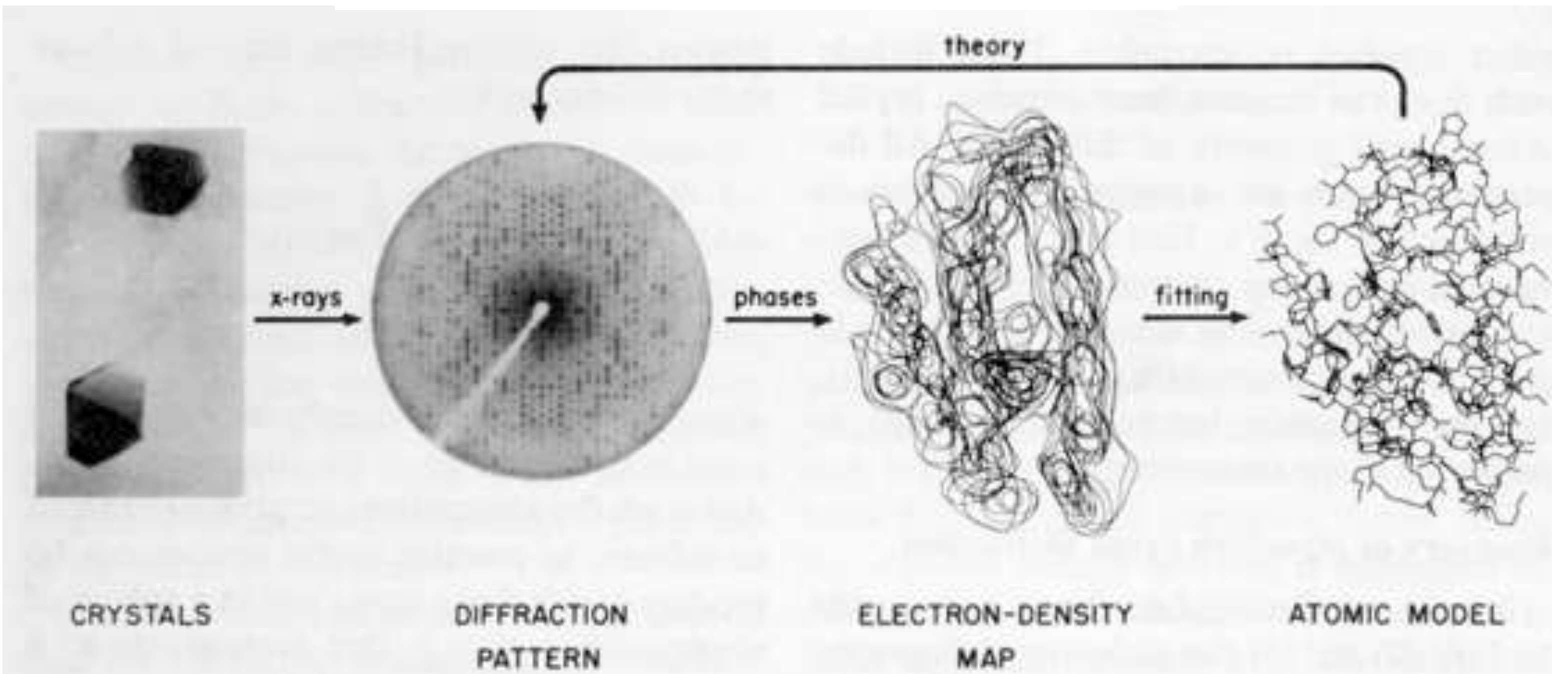
↓

Production of diffraction pattern of regularly spaced spots

↓

The 2-D images taken at different rotation are converted to 3-D models of the electron density map by the method of Fourier Transform


screen
X-ray
Crystal
diffracted ray


theory
x-rays
phases
fitting
CRYSTALS
DIFFRACTION
PATTERN
ELECTRON-DENSITY
MAP
ATOMIC MODEL

Applications of X-Ray Diffraction

- Find structure to determine function of proteins
- Convenient three letter acronym: XRD
- Distinguish between different crystal structures with identical compositions
- Study crystal deformation and stress properties
- Study of rapid biological and chemical processes

HIV-

Scientists also determined the X-ray crystallographic structure of HIV protease, a viral enzyme critical in HIV's life cycle, in 1989.

Pharmaceutical scientists hoped that by blocking this enzyme, they could prevent the virus from spreading in the body.

By feeding the structural information into a computer modeling program, they could use the model structure as a reference to determine the types of molecules that might block the enzyme.

Arthritis-

To create an effective painkiller in case of arthritis that doesn't cause ulcers, scientists realized they needed to develop new medicines that shut down COX-2 but not COX-1.

Through structural biology, they could see exactly why Celebrex plugs up COX-2 but not COX-1

References

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All the original contributors of the concept and findings published are gratefully acknowledged while preparing the e-content for the students of Biochemistry and allied sciences.