

X RAY WAVE INTERFERENCE AND CRYSTALLOGRAPHY**Ashutosh Dwivedi**Deputy Controller of Examinations
APJ Abdul Kalam Technical University Lucknow U.P**Abstract:**

X-ray **wave interference** (Roentgenstrahlinterferenzen), commonly known as X-ray diffraction (XRD), and was direct evidence for the periodic atomic structure of crystals postulated for several centuries:

Keywords:

Interference ray, XRD, diffraction

INTRODUCTION

The hypothesis is to imagine Bragg's diffraction as a reflection of X-rays on the surface of imaginary "mirrors" formed by atomic planes in the crystal lattice (shown as horizontal lines containing scattering centers, that is, atoms shown as blue circles in the left image). Due to the repetitive nature of the crystal, these planes would be separated by a constant distance **d**.

The two X-ray beams of wavelength λ , arrive in phase onto the respective imaginary planes, with an angle of incidence θ , and form a wave front (green line on the left).

In order to obtain a cooperative effect, after reflection both X-ray beams should still be in phase (green line on the right), a situation that will only happen if the difference of path travelled by the wave fronts **OF** and **OH** (wavefronts before and after reflection) corresponds with an integer number of wavelengths.

This condition is equivalent to say that the sum of the **FG** and **GH** segments corresponds to an integer (**n**) times the wavelength (λ):

$$\mathbf{FG + GH = n \cdot \lambda} \quad (1)$$

but $\mathbf{FG = GH}$ and $\mathbf{\sin \theta = FG / d}$

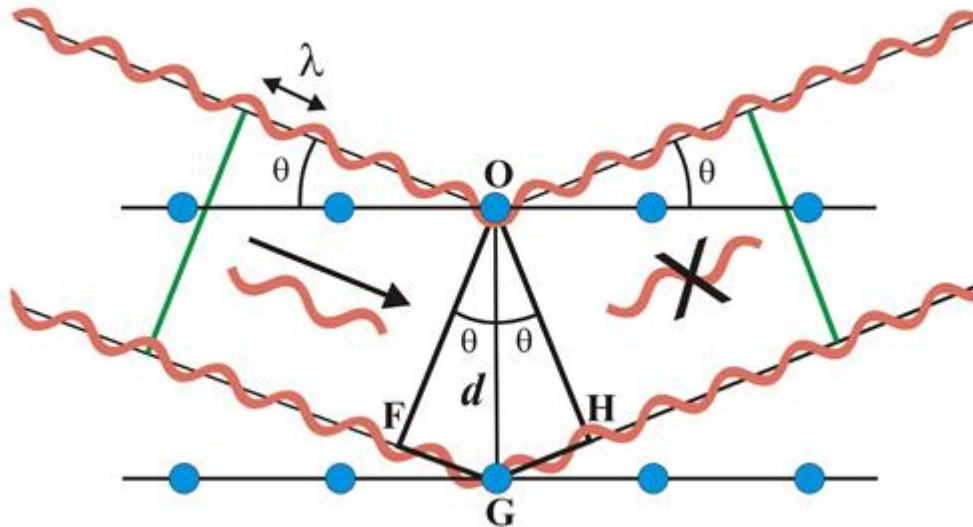
that is: $\mathbf{FG = d \sin \theta}$

and therefore expression (1) becomes:

$$\mathbf{2 d \sin \theta = n \cdot \lambda}$$

This is the **Bragg's Law**.

If the emerging reflected waves have opposite phase, no reflected intensity will be observed, ie, Bragg's Law is not fulfilled.



When the angle of incidence of the X-rays does not satisfy the Bragg's Law, the emergent beams are no longer in phase (green line on the right), and cancel each other, so that no reflected intensity will be observed.

If we consider the baseline scenario and look carefully at the Bragg's equation, it is easy to realize that:

- The lattice planes behave like mirrors reflecting the 'X-light' only in certain positions given by:

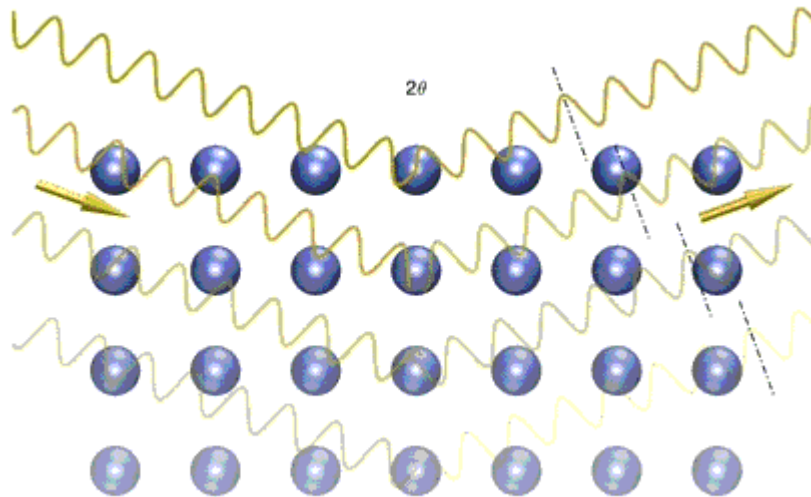
$$\theta = \sin^{-1} (n \cdot \lambda / 2 \cdot d)$$

- For given experimental conditions (λ and d) only discrete values of the diffraction angle θ are obtained, that correspond to the different values of the integer n .
- There are only a finite number of diffraction orders (as $\sin \theta \leq 1$) and the maximum number of them depends on the given experimental conditions (crystal and wavelength):

$$n_{\max} = 2 \cdot d / \lambda$$

- The geometry of diffraction (ie the diffraction angle θ) depends on the lattice geometry only.

The following animated gif gives an idea of what has been explained above. When the orientation of the incoming waves, always in phase (left), meet the above mentioned geometric conditions respect to the virtual atomic planes, the "reflected" X-ray waves will be in phase (right part of the animation), in which case the Bragg maximum (central peak of the image) is produced...



The Bragg condition is satisfied when the reflected waves are in phase

Bragg's Law refers to the simple equation:

$$(eq 1) \quad n\lambda = 2d \sin\theta$$

derived by the English physicists Sir W.H. Bragg and his son Sir W.L. Bragg in 1913 to explain why the cleavage faces of crystals appear to reflect X-ray beams at certain angles of incidence (theta, θ). The variable d is the distance between atomic layers in a crystal, and the variable λ is the **wavelength** of the incident X-ray beam (see applet); n is an integer

This observation is an example of X-ray **wave interference** (Roentgenstrahlinterferenzen), commonly known as X-ray diffraction (XRD), and was direct evidence for the periodic atomic structure of crystals postulated for several centuries. The Braggs were awarded the Nobel Prize in physics in 1915 for their work in determining crystal structures beginning with NaCl, ZnS and diamond. Although Bragg's law was used to explain the interference pattern of X-rays scattered by crystals, diffraction has been developed to study the structure of all states of matter with any beam, e.g., ions, electrons, neutrons, and protons, with a wavelength similar to the distance between the atomic or molecular structures of interest.

The applet shows two rays incident on two atomic layers of a crystal, e.g., atoms, ions, and molecules, separated by the distance d . The layers look like rows because the layers are projected onto two dimensions and your view is parallel to the layers. The applet begins with the scattered rays in phase and interfering constructively. Bragg's Law is satisfied and diffraction is occurring. The meter indicates how well the phases of the two rays match. The small light on the meter is green when Bragg's equation is satisfied and red when it is not satisfied.

The meter can be observed while the three variables in Bragg's are changed by clicking on the scrollbar arrows and by typing the values in the boxes. The d and θ variables can be changed by dragging on the arrows provided on the crystal layers and scattered beam, respectively.

Deriving Bragg's Law

Bragg's Law can easily be derived by considering the conditions necessary to make the phases of the beams coincide when the incident angle equals and reflecting angle. The rays of the incident beam are always in phase and parallel up to the point at which the top beam strikes the top layer at atom z (Fig.

1). The second beam continues to the next layer where it is scattered by atom B. The second beam must travel the extra distance $AB + BC$ if the two beams are to continue traveling adjacent and parallel. This extra distance must be an integral (n) multiple of the wavelength (λ) for the phases of the two beams to be the same:

(eq 2) $n\lambda = AB + BC .$

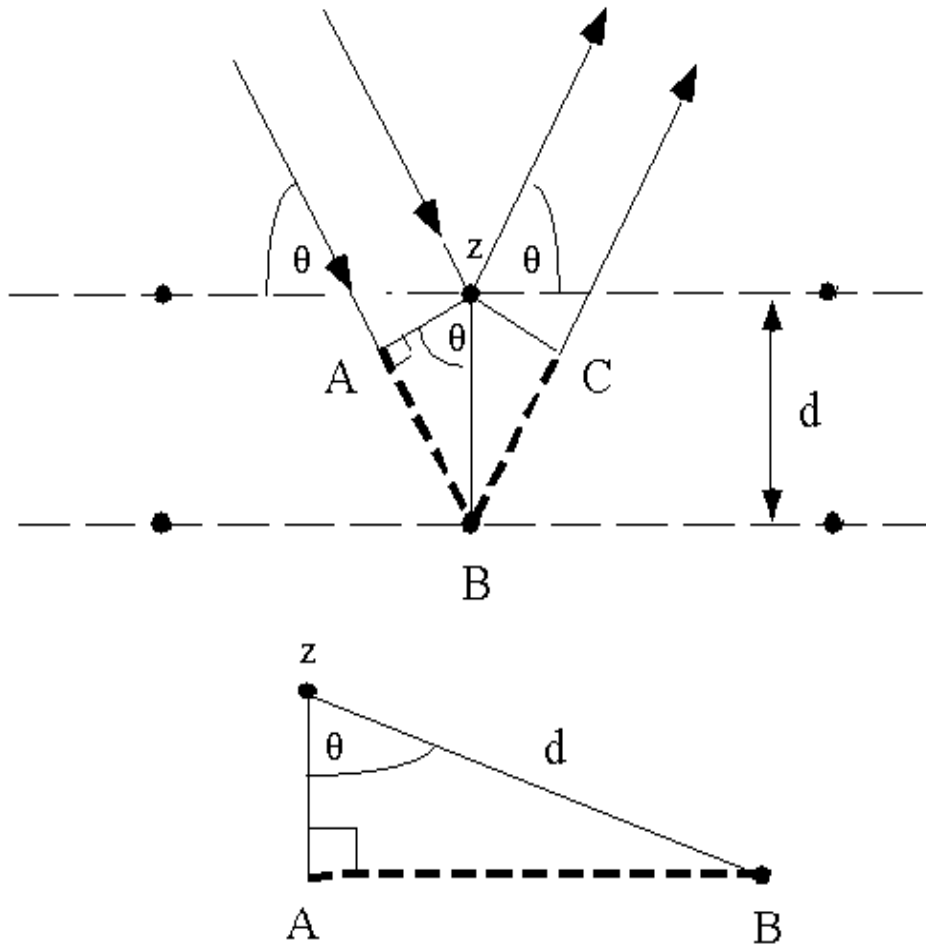


Fig. 1 Deriving Bragg's Law using the reflection geometry and applying trigonometry. The lower beam must travel the extra distance ($AB + BC$) to continue traveling parallel and adjacent to the top beam.

Recognizing d as the hypotenuse of the right triangle Abz , we can use trigonometry to relate d and θ to the distance ($AB + BC$). The distance AB is opposite θ so,

(eq 3) $AB = d \sin\theta .$

Because $AB = BC$ eq. (2) becomes,

(eq 4) $n\lambda = 2AB$

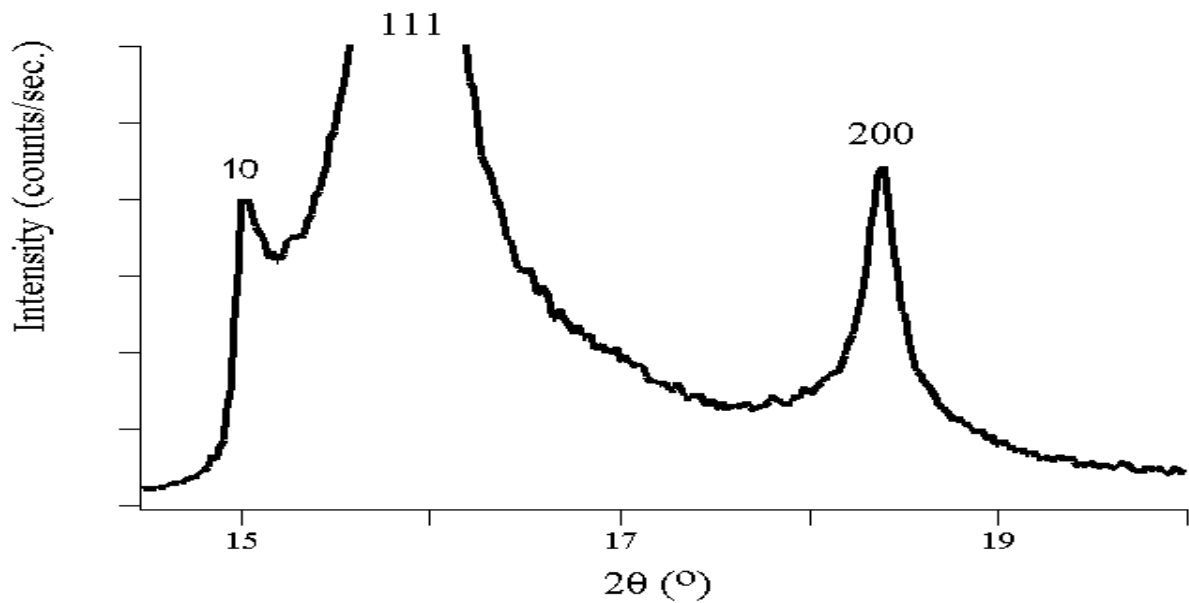
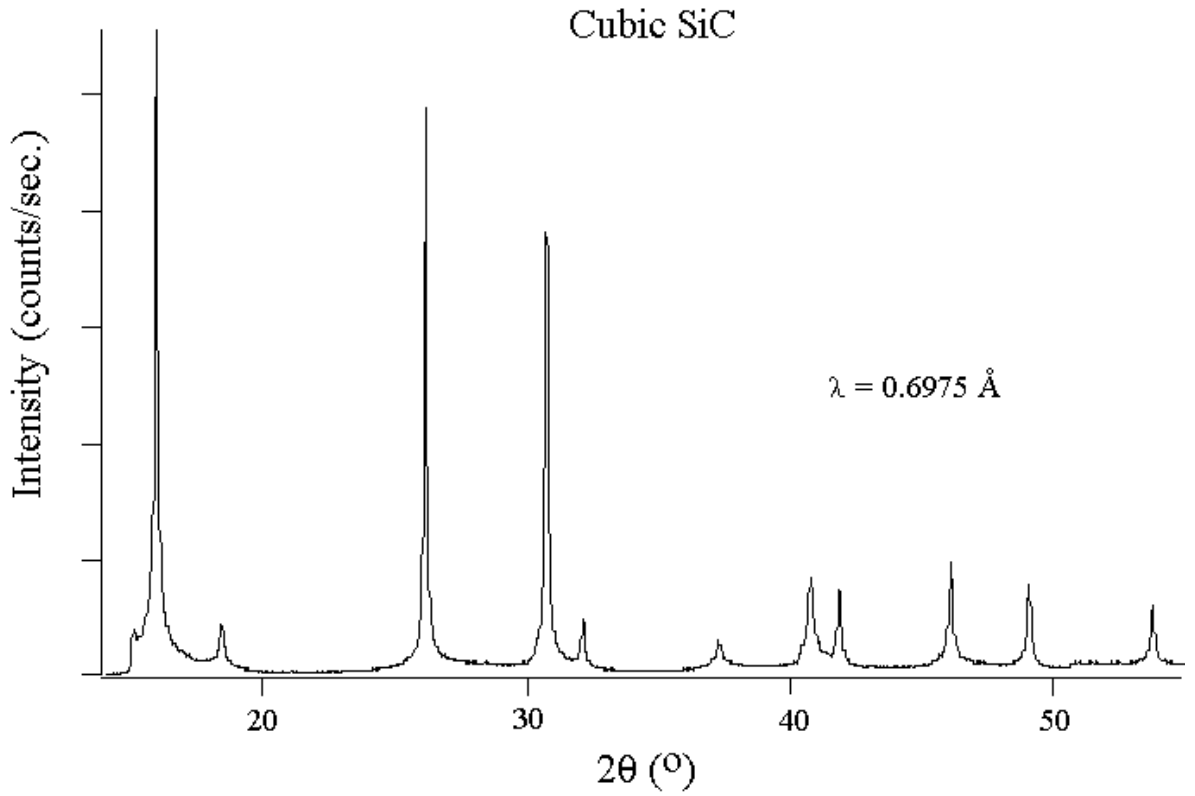
Substituting eq. (3) in eq. (4) we have,

(eq 1) $n\lambda = 2 d \sin\theta$

and Bragg's Law has been derived. The location of the surface does not change the derivation of Bragg's Law.

Experimental Diffraction Patterns

The following figures show experimental x-ray diffraction patterns of cubic SiC using synchrotron radiation.



Players in the Discovery of X-ray Diffraction

Friedrich and Knipping first observed Roentgenstrahlinterferenzen in 1912 after a hint from their research advisor, Max von Laue, at the University of Munich. Bragg's Law greatly simplified von Laue's description of X-ray interference. The Braggs used crystals in the reflection geometry to analyze the intensity and wavelengths of X-rays (spectra) generated by different materials. Their apparatus for characterizing X-ray spectra was the Bragg spectrometer.

Laue knew that X-rays had wavelengths on the order of 1 Å. After learning that Paul Ewald's optical theories had approximated the distance between atoms in a crystal by the same length, Laue postulated that X-rays would diffract, by analogy to the diffraction of light from small periodic scratches drawn on a solid surface (an optical diffraction grating). In 1918 Ewald constructed a theory, in a form similar to his optical theory, quantitatively explaining the fundamental physical interactions associated with XRD. Elements of Ewald's eloquent theory continue to be useful for many applications in physics.

If we use X-rays with a wavelength (λ) of 1.54Å, and we have diamonds in the material we are testing, we will find peaks on our X-ray pattern at θ values that correspond to each of the d-spacings that characterize diamond. These d-spacings are 1.075Å, 1.261Å, and 2.06Å. To discover where to expect peaks if diamond is present, you can set λ to 1.54Å in the applet, and set distance to one of the d-spacings. Then start with θ at 6 degrees, and vary it until you find a Bragg's condition. Do the same with each of the remaining d-spacings. Remember that in the applet, you are varying θ , while on the X-ray pattern printout, the angles are given as 2θ . Consequently, when the applet indicates a Bragg's condition at a particular angle, you must multiply that angle by 2 to locate the angle on the X-ray pattern printout where you would expect a peak

X-ray crystallography is a tool used for determining the atomic and molecular structure of a crystal. The underlying principle is that the crystalline atoms cause a beam of X-rays to diffract into many specific directions. By measuring the angles and intensities of these diffracted beams, a crystallographer can produce a 3D picture of the density of electrons within the crystal. From this electron density image, the mean positions of the atoms in the crystal can be determined, as well as their chemical bonds, their disorder, and various other information. The method revealed the structure and function of many biological molecules, including vitamins, drugs, proteins, and nucleic acids, such as DNA. Note that the double helix structure of DNA discovered by James Watson and Francis Crick was revealed by X-ray crystallography. Recent advances in image reconstruction technology have made X-ray crystallography amenable to the structural analysis of much larger complexes, such as virus particles (Fig. 2.11). The major shortcoming of X-ray crystallography is that it is difficult to obtain a crystal of virus particles, which is a prerequisite for X-ray crystallography. Another shortcoming is that X-ray crystallography generally requires placing the samples in nonphysiological environments, which can occasionally lead to functionally irrelevant conformational changes.

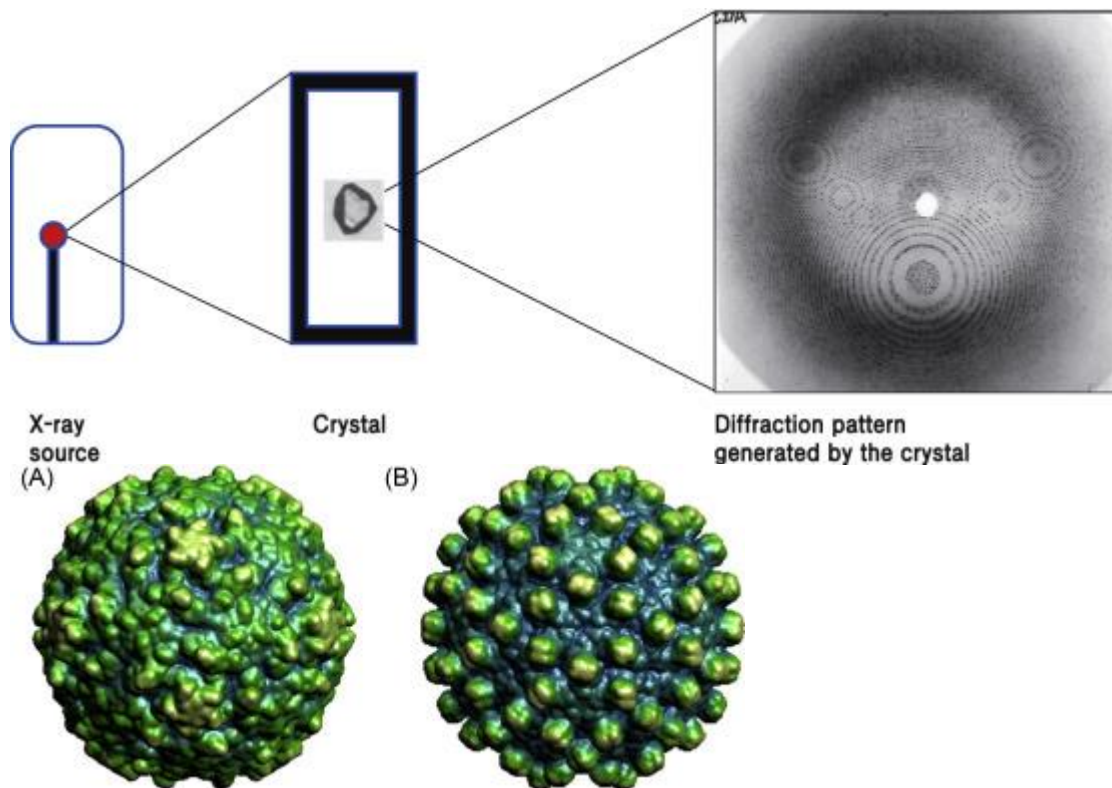


Fig-2Virus structure in high resolution

Conclusion; X-ray crystallography is a tool used for determining the atomic and molecular structure of a crystal. The underlying principle is that the crystalline atoms cause a beam of X-rays to diffract into many specific directions. By measuring the angles and intensities of these diffracted beams, a crystallographer can produce a 3D picture of the density of electrons within the crystal.

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2. See, for example, [this example calculation Archived](#) July 10, 2011, at the [Wayback Machine](#) of interatomic spacing with Bragg's law.
3. There are some sources, like the Academic American Encyclopedia, that attribute the discovery of the law to both W.L Bragg and his father W.H. Bragg, but the [official Nobel Prize site](#) and the biographies written about him ("Light Is a Messenger: The Life and Science of William Lawrence Bragg", Graeme K. Hunter, 2004 and "Great Solid State Physicists of the 20th Century", Julio Antonio Gonzalo, Carmen Aragón López) make a clear statement that Lawrence Bragg alone derived the law.
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