

**Bragg's law and XRD
(ModernPhysics)**

**e-content for B.Sc Physics (Honours)
B.Sc Part-II
Paper-IV**

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Bragg's Law

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

English physicists Sir W.H. Bragg and his son Sir W.L. Bragg developed a relationship 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 lambda λ is the **wavelength** of the incident X-ray beam; 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 Nobel Prize in Physics 1915

"for their services in the analysis of crystal structure by means of X-rays"

Bragg's Law

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



Sir William Henry Bragg

1/2 of the prize

United Kingdom

London University
London, United Kingdom

b. 1862
d. 1942



William Lawrence Bragg

1/2 of the prize

United Kingdom

Victoria University
Manchester, United Kingdom

b. 1890
(in Adelaide, Australia)
d. 1971

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.

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

Constructive interference occurs only when

$$n\lambda = AB + BC$$

$$AB = BC$$

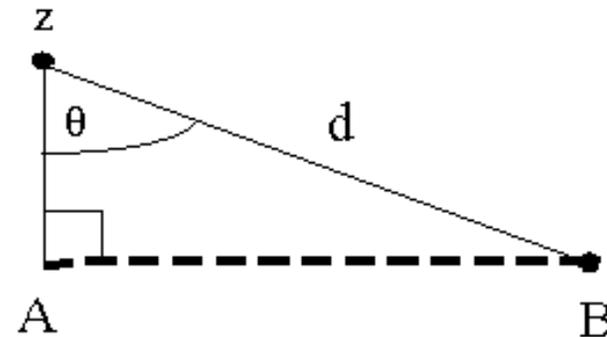
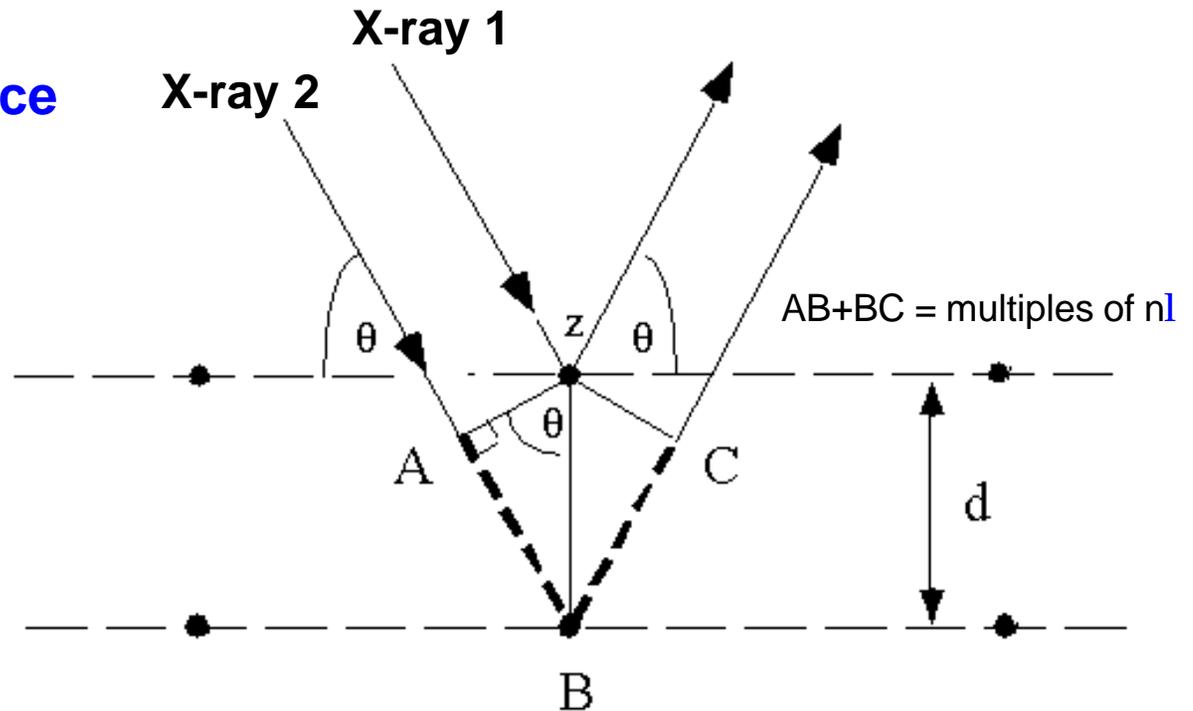
$$n\lambda = 2AB$$

$$\sin\theta = AB/d$$

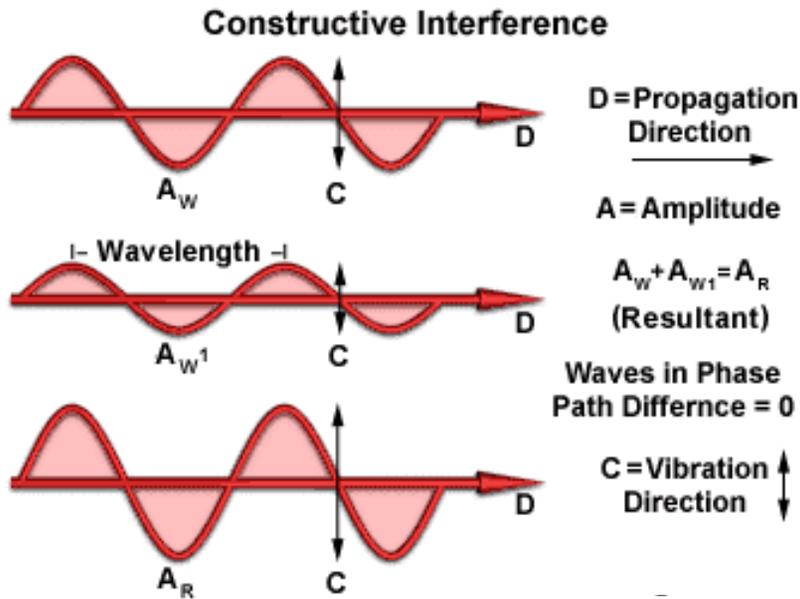
$$AB = d\sin\theta$$

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

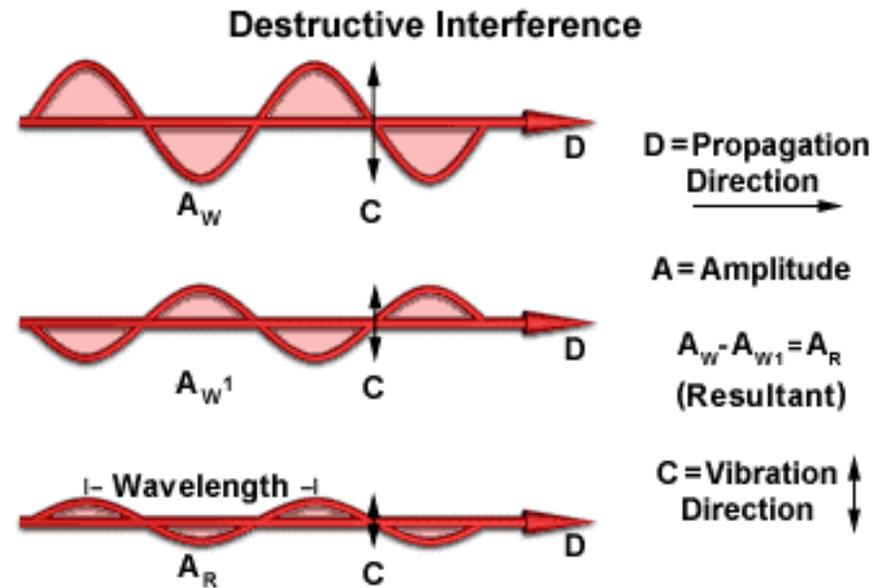
$$\lambda = 2d_{hkl}\sin\theta_{hkl}$$



Constructive and Destructive Interference of Waves



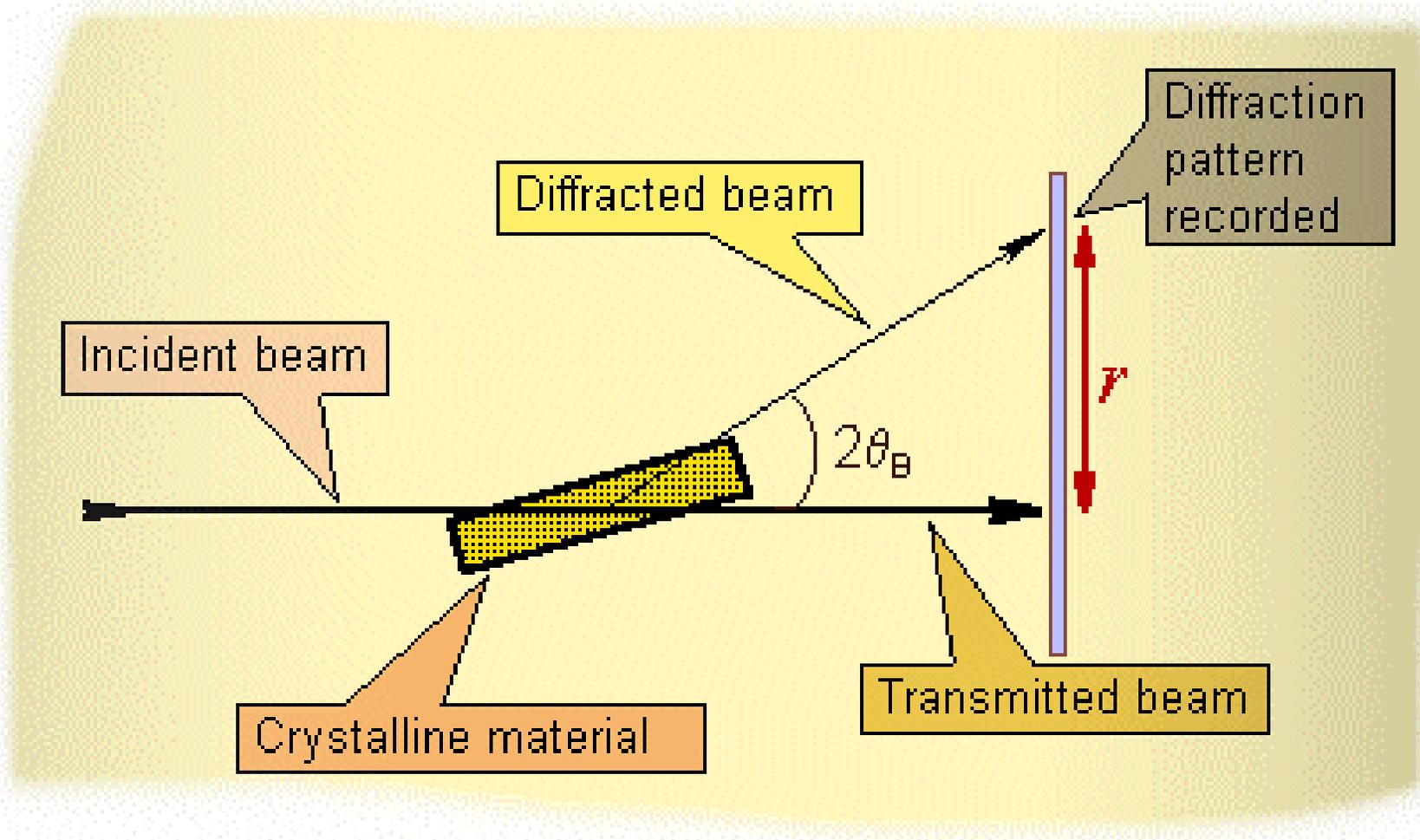
Constructive Interference
In Phase



Destructive Interference
Out of Phase

1.0 What is X-ray Diffraction ?

I

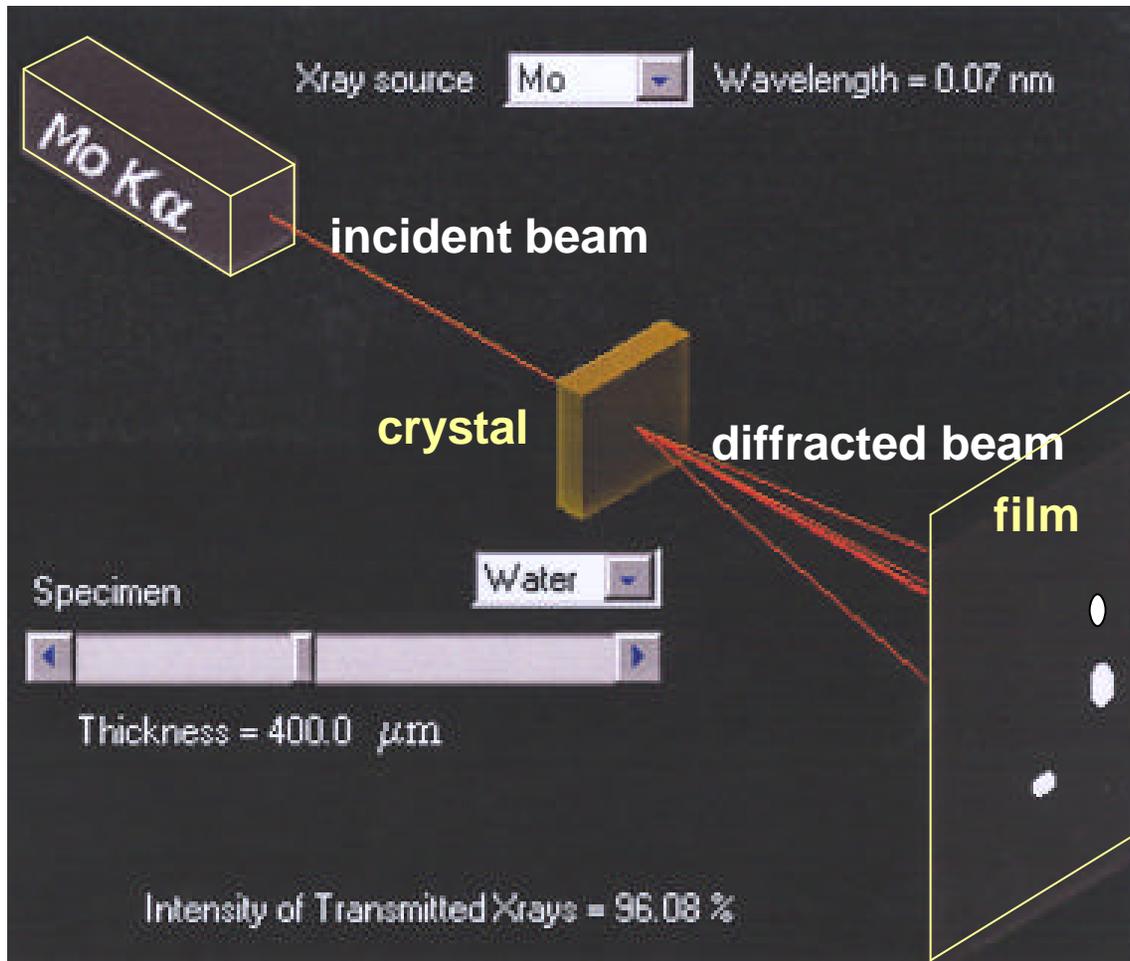


Why XRD?

- **Measure the average spacings between layers or rows of atoms**
- **Determine the orientation of a single crystal or grain**
- **Find the crystal structure of an unknown material**
- **Measure the size, shape and internal stress of small crystalline regions**

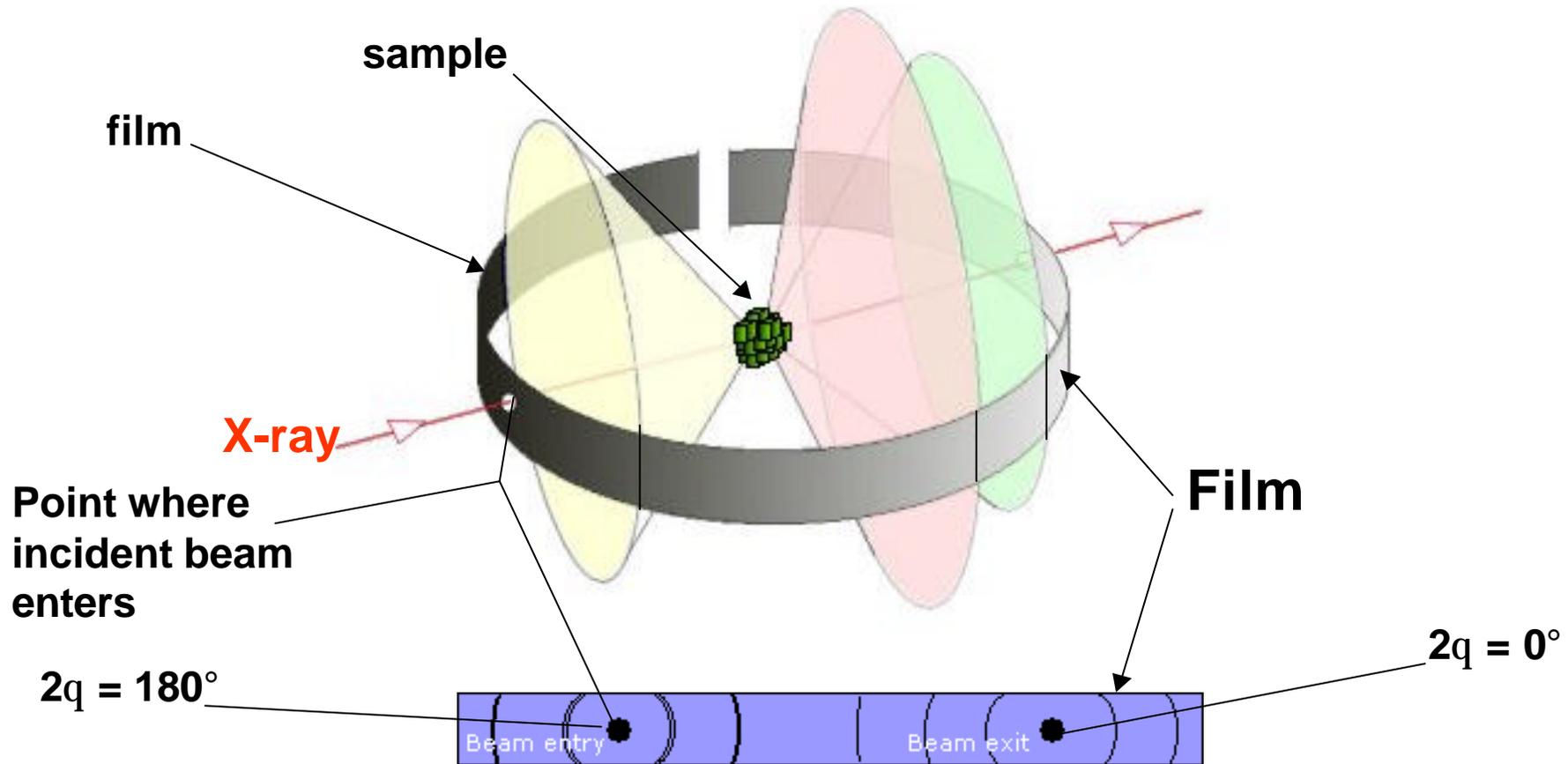
X-ray Diffraction (XRD)

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.



Effect of sample thickness on the absorption of X-rays

Detection of Diffracted X-rays by Photographic film



Debye - Scherrer Camera

A sample of some hundreds of crystals (i.e. a powdered sample) show that the diffracted beams form continuous cones. A circle of film is used to record the diffraction pattern as shown. Each cone intersects the film giving diffraction lines. The lines are seen as arcs on the film.

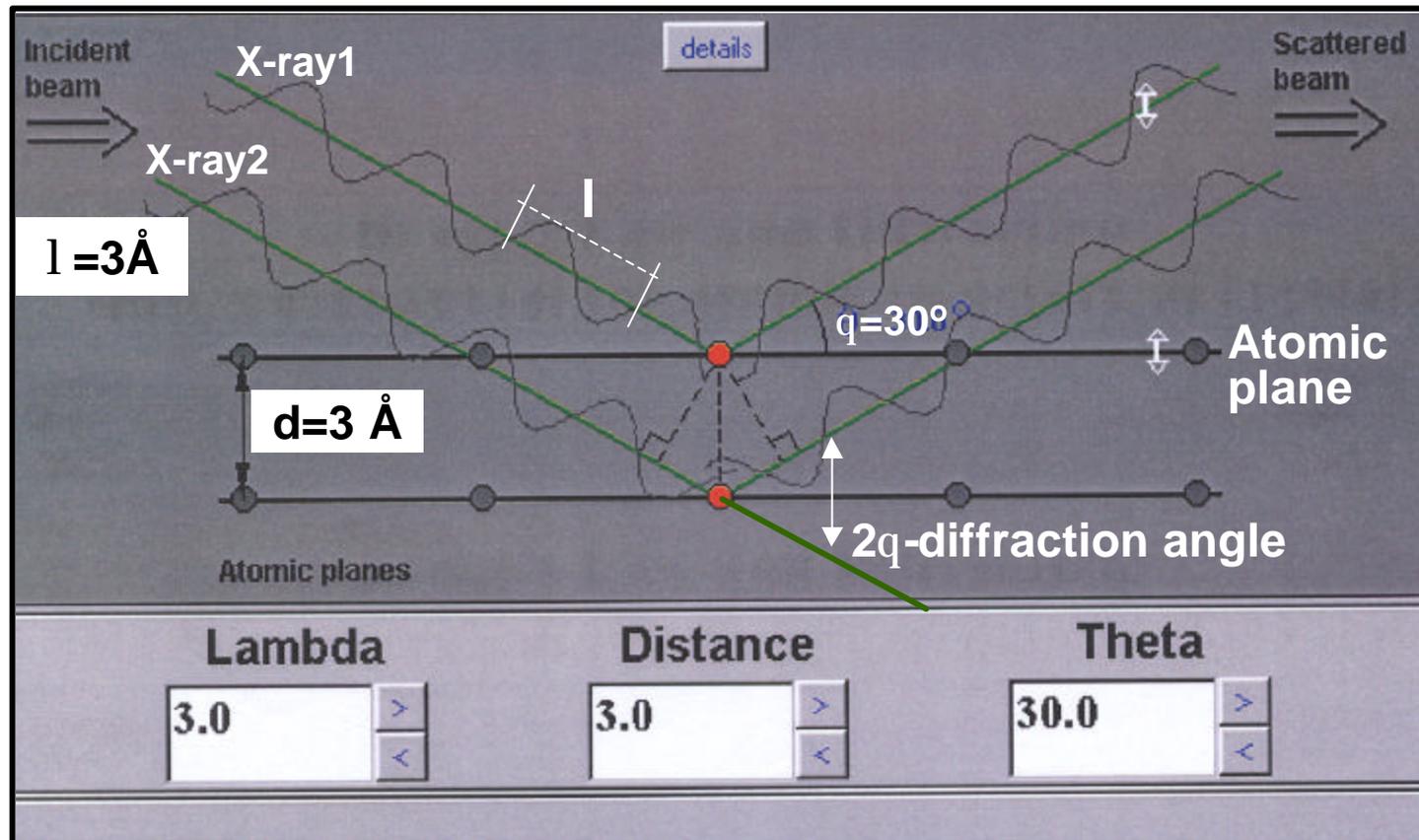
Bragg's Law and Diffraction:

How waves reveal the atomic structure of crystals

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

n-integer

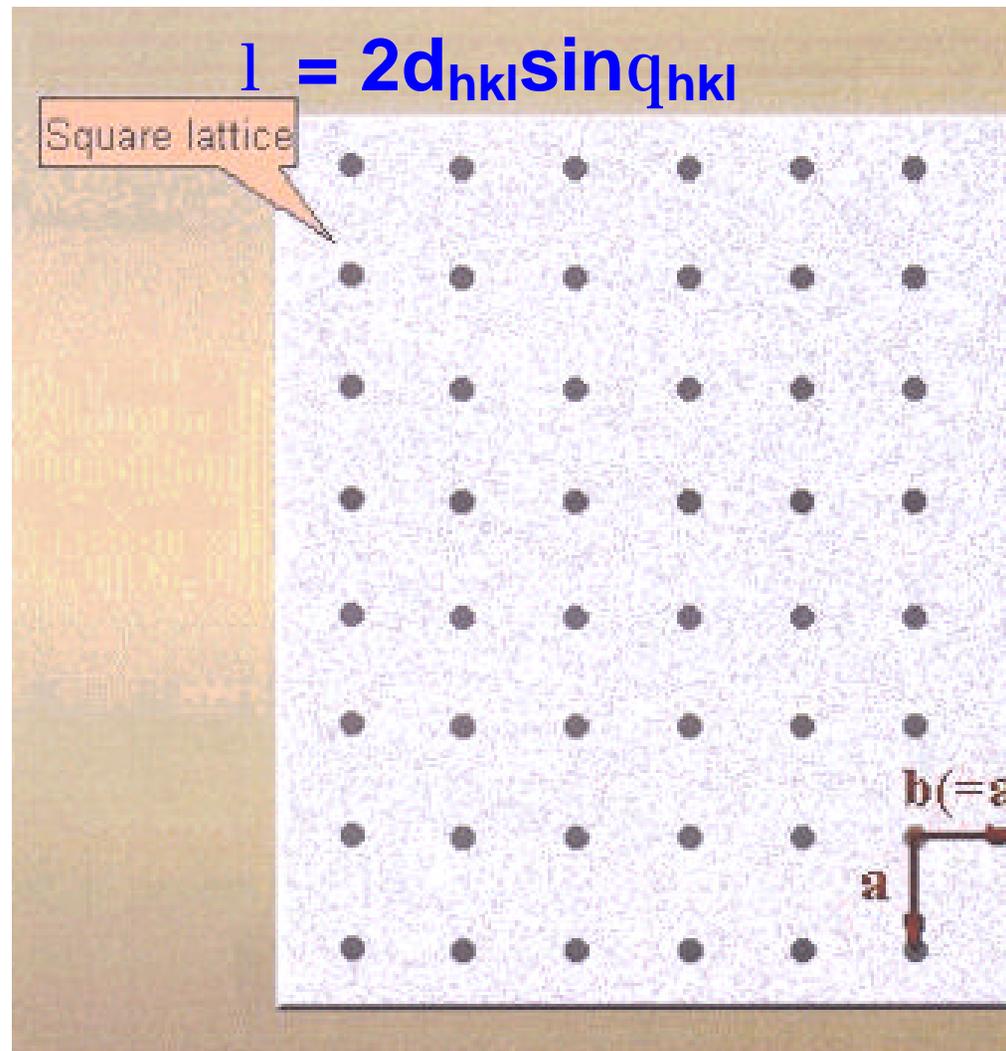
Diffraction occurs only when Bragg's Law is satisfied Condition for constructive interference (X-rays 1 & 2) from planes with spacing d



<http://www.eserc.stonybrook.edu/ProjectJava/Bragg/>

Planes in Crystals-2 dimension

Different planes
have different
spacings



To satisfy Bragg's Law, q must change as d changes
e.g., q decreases as d increases.