X-ray Crystallography (theory)

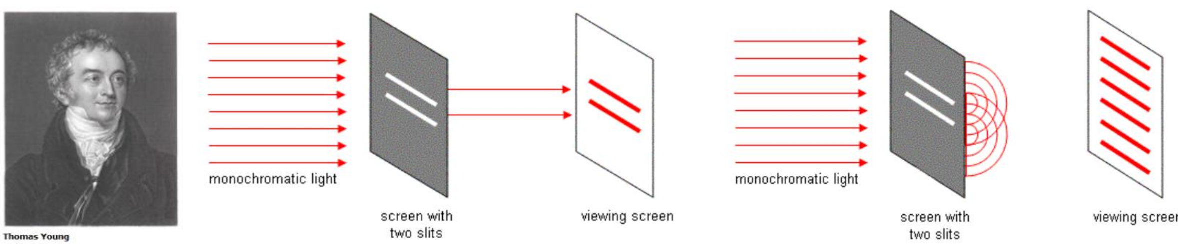
http://iycr2014.org/

To understand the X-rays as waves and the beginnings of X-ray crystallography, one needs to understand two key properties of waves – ***diffraction*** and ***interference***.

Diffraction: Diffraction refers to phenomena that occur when a wave encounters an obstacle, such as the apparent bending of waves around small obstacles and the spreading out of waves past small openings. Diffraction occurs with all waves, including sound waves, water waves, and electromagnetic waves such as visible light, X-rays, and radio waves. Diffraction effects are most pronounced for waves where the wavelength is roughly similar to the dimensions of the diffracting objects.

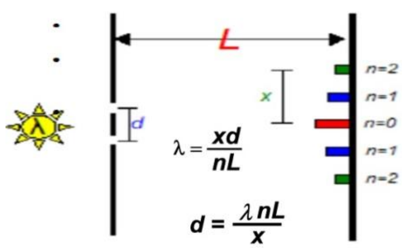
Interference: Interference is a phenomenon in which two waves superimpose to form a resultant wave of greater (constructive interference) or lower (destructive interference) amplitude.

These properties were used by Young in 1801 to show that light was made of waves instead of particles.



If light is a particle ….. **If light is a wave …..**

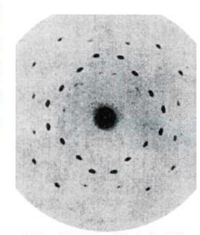
In 1912 Max von Laue proposed that if X-rays were short wavelength waves, then if a crystal were exposed to short wavelength X-ray waves, the small spacings in crystals should result in a "diffraction / interference" pattern of "spots". If the wavelength is known, then the spacing of the spots can be used to calculate the dimensions of the unit cell in the crystals (e.g. *a, b, c*)!



λ = wavelength of light used (m)
x = distance from central fringe (m)
d = distance between the slits (m)
n = the order of the fringe
L = length from the screen with slits to the viewing screen (m)

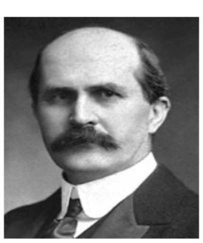
$$\lambda = \frac{2d\sin\theta}{n} \quad \text{or} \quad d = \frac{n\lambda}{2\sin\theta}$$

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



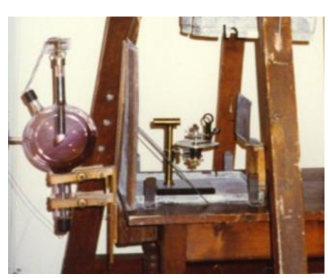
Max Laue's photo of X-ray diffraction from ZnS revealed spots of varying shape and intensity.

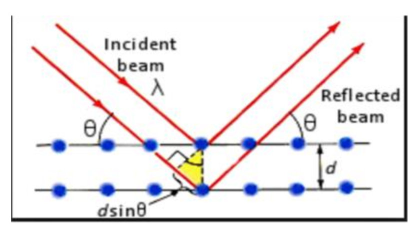
William Lawrence Bragg realized that the intensity of the "spots" could be combined with the distance information to determine the structural arrangement of the atoms in the crystals. In 1913, young Bragg and his father determined the first crystal structures of NaCl, diamond, etc. Note the reciprocal relationship of "d" and "sinθ" in Bragg's Law.



Sir William Henry Bragg

William Lawrence Bragg





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

Max von Laue was awarded the 1914 Nobel Prize for his work, and the Braggs the 1915 Nobel Prize for their contributions. William Lawrence Bragg was just 25 years old when he won the Nobel Prize!

Optical Transforms (demos)

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With a laser pointer and a “diffraction” slide, it is possible to demonstrate the ***reciprocal relationship*** of “d” and “sinθ” in Bragg’s Law ($\mathbf{n\lambda = 2dsin\theta}$) using optical transforms to visualize the relationship between wavelength and “sinθ” for the same crystal (“d”), or the effect of different arrangements of scatterers to produce different intensities in the optical transform patterns. There are also programs available online to calculate the transform of an object. It was this understanding of optical transforms that enabled Francis Crick and James Watson to quickly propose and build the double helix model of DNA after seeing the fiber diffraction pattern taken by Rosalind Franklin in Maurice Wilkens’ lab. http://escher.epfl.ch/fft/

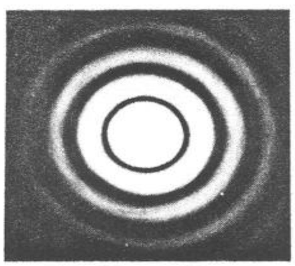
Below are a series of “objects” and their “optical transforms”. Note the reciprocal relationship, large objects and separations in real (object) space results in smaller separations in transform space. Also note that the transform of the object (●) is sampled by the transform of the lattice.

a) 

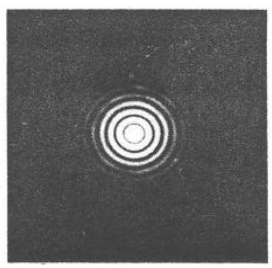
b) 

c) 

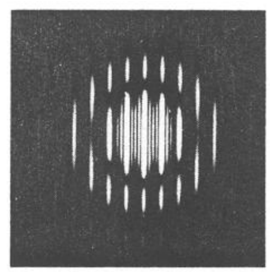
d) 



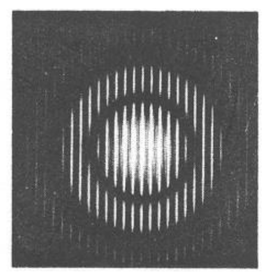
a



b

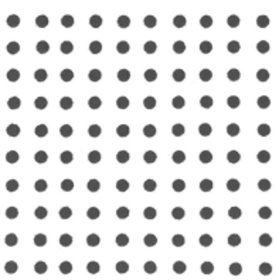


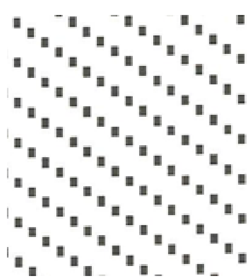
c

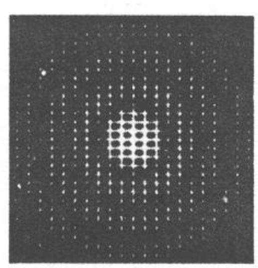


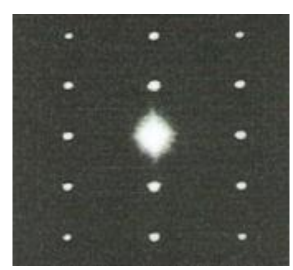
d

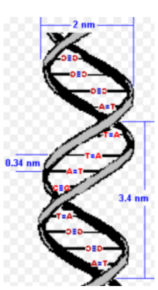
Below are four objects (e, f, g, h) and four transforms. Match the objects with their corresponding optical transforms by placing the appropriate letter on the blank provided (ref. Optical Transforms, H. Lipson; ICE, Univ. of Wisconsin; http://ice.chem.wisc.edu/)

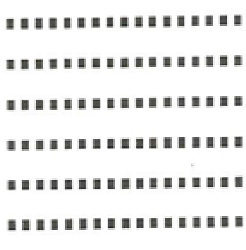
e) 

f) 

__ 

__ 

g) 

h) 

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