Bragg's law

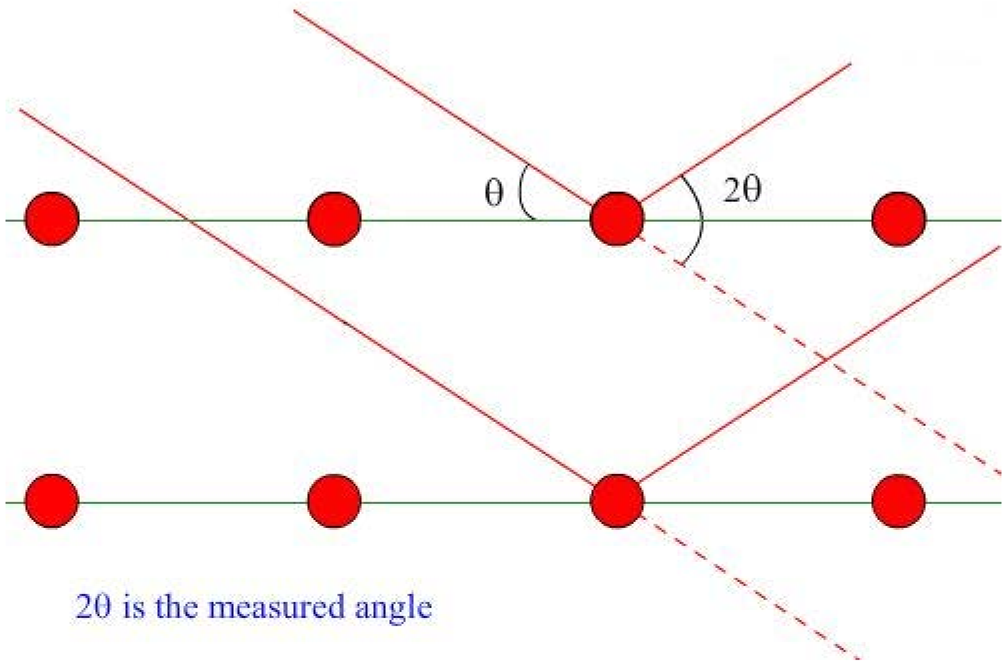
The concept used to derive Bragg's law is very similar to that used for Young's double slit experiment.

An X-ray incident upon a sample will either be transmitted, in which case it will continue along its original direction, or it will be scattered by the electrons of the atoms in the material. All the atoms in the path of the X-ray beam scatter X-rays.

We are primarily interested in the peaks formed when scattered X-rays constructively interfere. (In addition, after scattering some X-rays suffer a change in wavelength. This incoherent scattering is not considered here).

Constructive interference occurs when two X-ray waves with phases separated by an integer number of wavelengths add to make a new wave with a larger amplitude.

When two parallel X-rays from a coherent source scatter from two adjacent planes their path difference must be an integer number of wavelengths for constructive interference to occur.



Path difference = $n\lambda$

Therefore;

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

In order to consider the general case of hkl planes, the equation can be rewritten as:

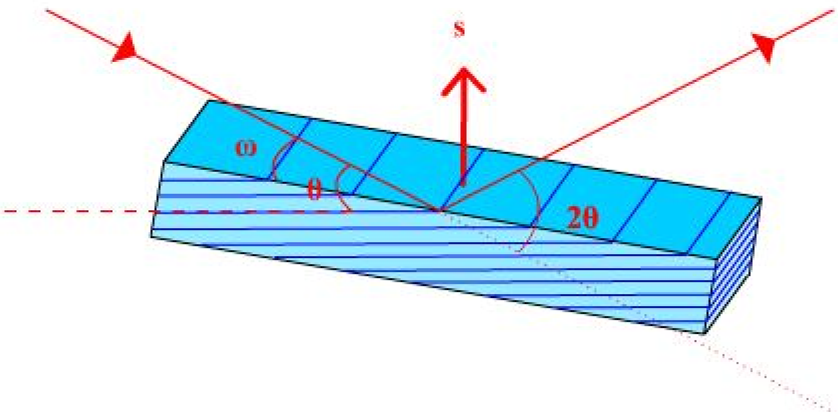
$\lambda = 2 d_{hkl} \sin\theta_{hkl}$

since the dhkl incorporates higher orders of diffraction i.e. n greater than 1.

The angle between the transmitted and Bragg diffracted beams is always equal to 2θ as a consequence of the geometry of the Bragg condition. This angle is readily obtainable in experimental situations and hence the results of X-ray diffraction are frequently given in terms of 2θ. However, it is very important to remember that the angle used in the Bragg equation must always be that corresponding to the angle between the incident radiation and the diffracting plane, i.e. θ.

The diffracting plane might not be parallel to the surface of the sample in which case the sample must be tilted to fulfil this condition. (The concept of orientation will be dealt with later in this TLP).

This is the procedure to obtain asymmetric reflections and work in transmission:

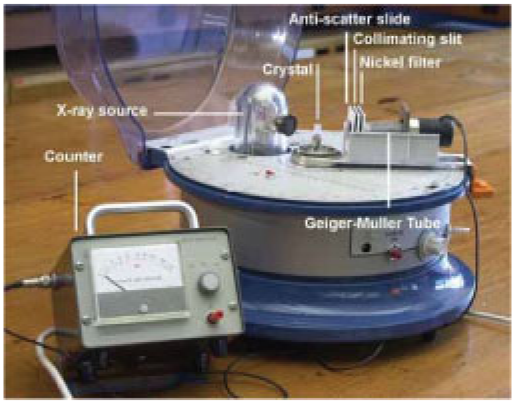


To measure the diffraction peak the sample is rotated by the offset. Now ω is not equal to θ. This is called an asymmetric reflection

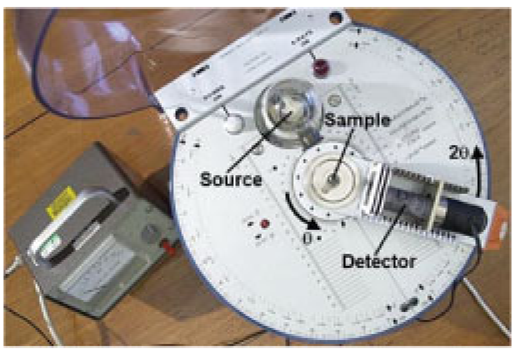
Single crystal diffraction:

The simplest way of demonstrating application of Bragg’s law is to diffract X-rays through a single crystal.

The simple teaching diffractometer in the photo below projects a beam of X-rays onto the crystal. The diffracted beam is collated through a narrow slit and passed through a nickel filter. The counter is a Geiger-Müller tube.



Diffractometer (Click on image to view larger version)



Top view of diffractometer (Click on image to view larger version)

The crystal used in this experiment is lithium fluoride. Assuming that the large flat face will be perpendicular to a particular crystallographic direction, this is set parallel to the line containing the source and detector at $\theta = 0$. The gearing of the counter arm is such that, once set, the θ - 2θ relationship between the incident, transmitted and diffracted beams is maintained.

The video below shows manual operation and the location of the first diffraction peak. Watch the counter carefully.
View video (30.77 MB) ... in separate window ... video alone

Using the 2θ value observed at a peak of intensity, the known wavelength λ for Cu Ka, = 1.54Å and the Bragg equation, a value for the plane spacing (d spacing) can be determined. If the peaks can be indexed, i.e. assigned to scattering from certain planes, then from simple geometry lattice parameters can be calculated. This is shown later in the TLP.

Source: http://www.doitpoms.ac.uk/tlplib/xray-diffraction/bragg.php