1.11: Bragg's Law

Bragg's law provides the condition for a plane wave to be diffracted by a family of lattice planes:

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

where d is the **lattice** spacing, θ the angle between the wavevector of the incident plane wave, $\mathbf{k_o}$, and the lattice planes, λ its wave length and n is an integer, the order of the reflection. It is equivalent to the diffraction condition in reciprocal space and to the Laue equations.

Direct Derivation of Bragg's Law

- **Reflection from the first plane:** The scattered waves will be in phase whatever the distribution of the point scatterers in the first plane if the angle of the reflected wave vector, $\mathbf{k_h}$, is also equal to θ. This is Snell-Descartes' law of reflection.
- **Reflection from the second plane:** Since the phase of the reflected waves is independent of the position of the point scatterer in the plane, the phase difference between the waves reflected by two successive lattice planes is obtained by choosing arbitrarily a scattering point, A, on the first plane and a scattering point, b on the second plane such that AB is normal to the planes. If C and d are the projections of A on the incident and reflected wave vectors passing through B, it is clear from Figure 1 that the path difference between the waves reflected at A and B, respectively, is:

$$CB + BD = 2d\sin\theta$$

  and that the two waves will be in phase if this path difference is equal to $n\,\lambda$ where n is an integer.
- **Reflection from the third, etc., planes:** If Bragg's relation is satisfied for the first two planes, the waves reflected with wave vector $\mathbf{k_h}$ will be in phase fo all the planes of the family.

Order of the Reflection

Bragg's law may also be written:

$$2(d/n)sin\theta = \lambda.$$

One may then say that a Bragg reflection of order n on a family of lattice planes or order n is equivalent to reflection of order 1 on a family of fictitious, or imaginary, planes of lattice spacing:

$$d_{hkl} = \frac{d}{n}$$

This fictitious family is associated to the reciprocal lattice vector **OH** where $OH = n/d = 1/d_{hkl}$. The indices of the reflection are:*hkl*. For instance, the dashed blue lines in Figure 1 correspond to the fistitious planes associated to the second order, $n = 2$.
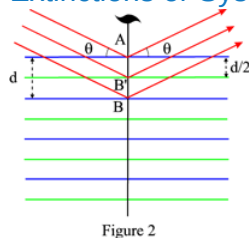
Extinctions or Systematic Absences

Figure 2

If there is a glide plane or a screw axis normal to the lattice planes, the spacing of the actual reflecting planes is $d/2$ for a glide plane and $(d\,p/q)$ for a q_p screw axis. Bragg's law should then be written:

$$2\left(\frac{d}{2}\right)\sin\theta = n\lambda$$

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

for a glide plane and

$$2(dp/q)\sin\theta = n\lambda \Rightarrow 2d\sin\theta = (q/p)n\lambda$$

for a screw axis q_p.

The reflections of odd order for a glide plane and of order different from $(q/p)n$ for a screw axis are then absent. One speaks of extinctions or systematic absences related to the presence of glide or screw components.

As an example, Figure 2 shows the case of a 2_1 screw axis: the reflecting planes are the blue planes and the green planes deduced from the latter by the action of the screw axis. Reflections of odd order will be sytematically absent.

Influence of deformation

A deformation that leaves a family of lattice planes (*hkl*) undistorted and its lattice spacing *d* unchanged will not affect the Bragg angle of *kkl* reflections, *e.g.* lattice planes parallel to a screw dislocations.

History

Bragg (1890-1971) presented his derivation of the reflection condition at a meeting of the Cambridge Philosophical Society on 11 November 1912. His paper was published in 1913 (Bragg W.L., 1913, *The Diffraction of Short Electromagnetic Waves by a Crystal*, *Proc. Cambridge Phil. Soc.*, **17**, 43-57. For details, see P. P. Ewald, 1962, IUCr, 50 Years of X-ray Diffraction, Section 5, page 64.