# X-Rays Diffraction (XRD)

**X-ray diffraction (XRD)** relies on the dual wave/particle nature of X-rays to obtain information about the **structure of crystalline materials**. A primary use of the technique is the identification and characterization of compounds based on their diffraction pattern.

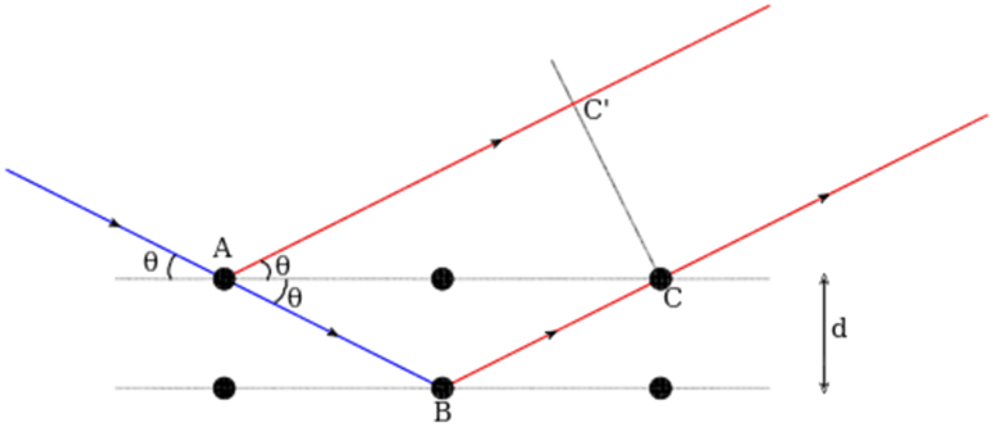
**The directions of possible diffractions depend on the size and shape of the unit cell of the material. The intensities of the diffracted waves depend on the kind and arrangement of atoms in the crystal Lattice.**

The diffraction of X-rays by crystals is described by Bragg's Law:

$$\mathbf{n\lambda = 2dsin\theta}$$

where ***n*** is a positive integer (0,1,2..), $\boldsymbol{\lambda}$ is the wavelength of the incident wave, **d** is interplanar distance an $\boldsymbol{\theta}$ **is glancing angle.**

# Derivation of Bragg's Law:




Suppose that a single monochromatic wave  is incident on aligned planes of lattice points, with separation **d,** at angle ϴ. Points **A** and **C** are on one plane, and **B** is on the plane below. Points **ABCC**' form a quadrilateral.

There will be a path difference between the ray that gets reflected along **AC'** and the ray that gets transmitted along **AB**, then reflected along **BC**. This path difference is:

# Derivation of Bragg's Law:

$(\mathrm{AB} + \mathrm{BC}) - (\mathrm{AC}')$..................................**1**

The two separate waves will arrive at a point with the same phase, and hence undergo **constructive interference**, if and only if this **path difference** is equal to any integer value of the **wavelength**, i.e.

$$n\lambda = (AB + BC) - (AC') \ldots\ldots\ldots\ldots\ldots\ldots.\ \mathbf{2}$$

# Derivation of Bragg's Law:

Therefore,

$\mathbf{AB = BC = \frac{d}{sin\theta}}$ and

$\mathbf{AC = \frac{2d}{tan\theta}}$

For which it follow that

$\mathbf{AC' = AC\ cos\theta = \frac{2d}{tan\theta}\ cos\Theta = \left(\frac{2d}{sin\theta}\ cos\theta\right) cos\theta = \frac{2d}{sin\theta}\ cos^2\Theta}$

Putting everything's together

$\boldsymbol{n\lambda = \frac{2d}{sin\theta} - \frac{2d}{sin\theta}cos^2\Theta = \frac{2d}{sin\theta}(1 - cos^2\theta) = \frac{2d}{sin\theta}sin^2\theta}$

which simplifies to

$\mathbf{n\lambda = 2dsin\Theta}$ *(which is Bragg's law.)*

Bragg's law, as stated above, can be used to obtain the lattice spacing of a particular cubic system through the following relation:

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

where **a** is the lattice spacing of the cubic crystal, **and h, k,** and **ℓ** are the Miller indices of the Bragg plane. Combining this relation with **Bragg's law** gives

$$\left(\frac{\lambda}{2a}\right)^2 = \left(\frac{\lambda}{2d}\right)^2 \frac{1}{h^2+k^2+l^2}$$

# Bragg's Law Selection Rule:

| Bravais lattices | Allowed reflections | Forbidden reflections |
|---|---|---|
| Simple cubic | Any h, k, ℓ | None |
| Body-centered cubic | h + k + ℓ = even | h + k + ℓ = odd |
| Face-centered cubic (FCC) | h, k, ℓ all odd or all even | h, k, ℓ mixed odd and even |

# Thank You