Module3

Laue diffraction, Laue equation, Ewald's sphere construction

Learning objectives

- Introduction
- Laue Diffraction
- Laue equations
- Bragg's Law from Laue equation
- Ewald's Sphere

3.1. Introduction

Laue used flat-plate film for recording the diffraction pattern of a stationary crystal when unfiltered X-rays are incident. In the Laue methods the Bragg equation is satisfied by effectively varying λ, utilizing the beam of continuous radiation. The crystal acts as a filter, selecting the correct wavelength for each reflection according to the equation $2d_{hkl}\sin\theta_{hkl} = \lambda$. From the Laue photographs, symmetries can be observed. Laue derived three equations as necessary conditions for producing diffraction pattern and Bragg's law can be derived from these equations.

3.2. Laue Diffraction

In 1912, von Laue took the diffraction pattern (Fig 3.1) when a still crystal is incident with a beam of continuous X-rays (unfiltered). The film used was a flat-plate one. The Laue photograph contains ellipses of varying intensities and the ellipses have one end of their major axis at the centre of the photographic film (Fig 3.2). The spots in each ellipse are due to reflections from planes that lie in one and the same zone. Fig 3.3 shows a zone axis Z' for a given Bragg angle θ. R can be considered as a reflected ray and if one imagines the rotation of the crystal about zone axis ZZ', taking the reflected beam with it we can simulate the effect of the zone. Now the rays like R generate a cone, co-axial with ZZ' with a semi vertical angle θ. Eventually, when a circle cuts a plane, the shape will be an ellipse and this is the reason why a general appearance of the spots of the Laue photographs are of ellipse in shape (refer Fig 3.2).

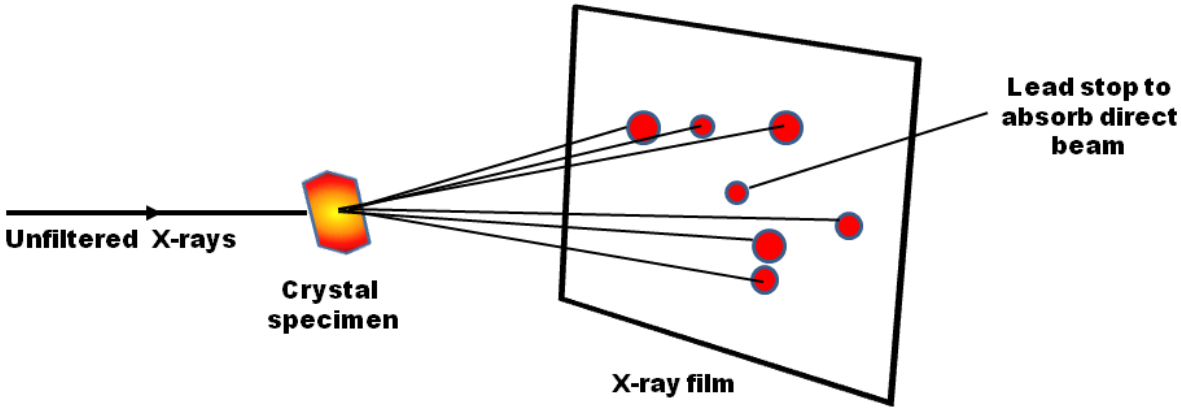

Fig 3.1

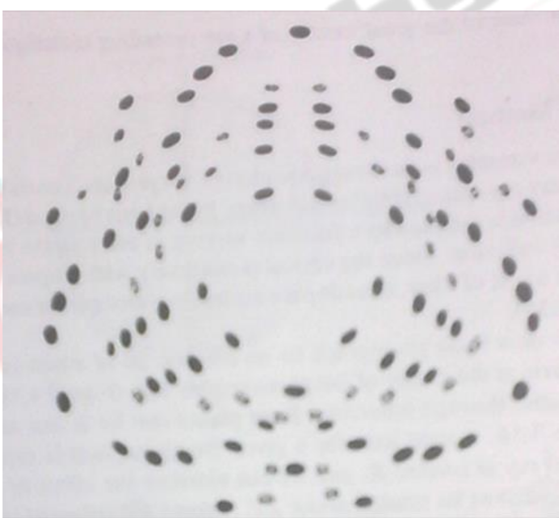

Fig 3.2

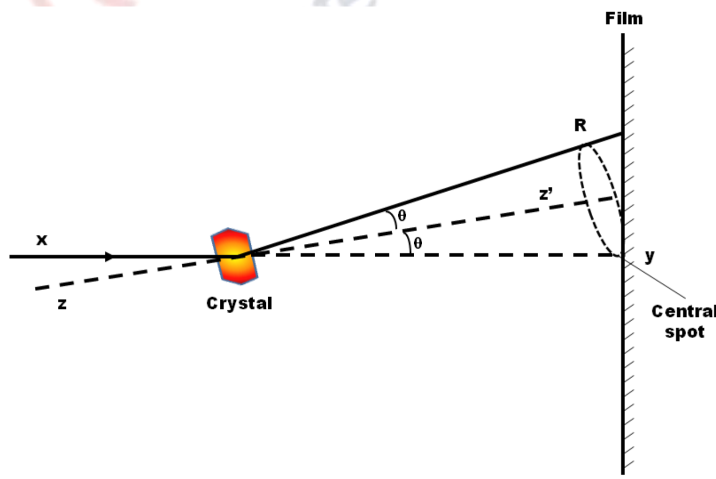

Fig 3.3

Since synchrotron uses a wide range of wavelengths, it is ideally suited to the Laue method of recording diffraction pattern.

3.3. Laue equations

Consider X-ray scattering by two atoms, one O and the other at A (Fig 3.4). O is considered as origin of the crystal lattice and the scattering of X-rays by O is affected by those scattered by atom 'A' whose coordinates with respect to O are at $p\mathbf{a_1}$, $q\mathbf{a_2}$, $r\mathbf{a_3}$, where **p, q and r** are integers. Thus

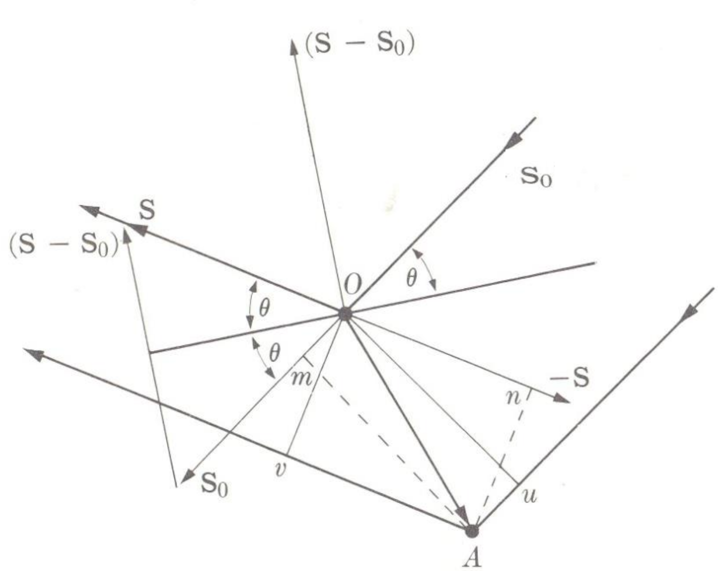

Fig 3.4

$$OA = p\mathbf{a_1} + q\mathbf{a_2} + r\mathbf{a_3} \qquad (3.1)$$

Where $\mathbf{a_1}$, $\mathbf{a_2}$ and $\mathbf{a_3}$ are the vectors defining the unit cell of the crystal lattice.

Assume λ is the wavelength of X-rays and let $\boldsymbol{S_o}$ and $\boldsymbol{S}$ be the unit vectors that represent the incident and diffracted beams, respectively. $\boldsymbol{S_o}$, $\boldsymbol{S}$ and **OA** in general are not coplanar.

We are now interested in the conditions under which diffraction will occur. For this, one has to determine the phase difference between the rays scattered by the atom O and A. Ou and Ov are wave fronts perpendicular to the incident beam and the scattered beam, respectively. Let δ be the path difference of the rays scattered by O and A. Let

$$\delta = uA + Av = Om + On = \boldsymbol{S_o}\,.\boldsymbol{OA} + (-\boldsymbol{S}).\boldsymbol{OA} = -\boldsymbol{OA}.(\boldsymbol{S} - \boldsymbol{S_o}) \qquad (3.2)$$

Path difference of λ corresponds to a phase difference of 2π radians and hence the corresponding phase difference ϕ, in radians for the above path difference δ , is given by

$$\phi = \frac{2\pi\delta}{\lambda} = -2\pi\left(\frac{\boldsymbol{S} - \boldsymbol{S_0}}{\lambda}\right).\boldsymbol{OA} \qquad (3.3)$$

Diffraction is now related to the reciprocal lattice by expressing the vector $(\boldsymbol{S} - \boldsymbol{S_o}/\lambda)$ as a vector in that lattice. Let

$$\left(\frac{\boldsymbol{S}-\boldsymbol{S_o}}{\lambda}\right) = h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3} \qquad (3.4)$$

Where $\mathbf{b_1}$, $\mathbf{b_2}$ and $\mathbf{b_3}$ are the unit cell translations of the reciprocal lattice

The above equation is now in the form of a vector in the reciprocal space but, at this point, no particular significance is attached to the parameters $h, k\ and\ l$. They are continuous variables and may assume any values, integral or nonintegral. Substituting equation (3.1) (for **OA**) and equation (3.4) [for $\left(\frac{\boldsymbol{S}-\boldsymbol{S_o}}{\lambda}\right)$], equation (3.3) now becomes

$$\boldsymbol{\phi} = -\boldsymbol{2\pi}(h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3}).(p\boldsymbol{a_1} + q\boldsymbol{a_2} + r\boldsymbol{a_3}) = -2\pi(hp + kq + lr) \qquad (3.5)$$

A diffracted beam will be found only if reinforcement occurs, and this requires that ϕ be an integral multiple of 2π, meaning that $hp + kq + lr$ should be an integer for obtaining a diffracted beam. This can happen only if $h, k\ and\ l$ are the integers as already p, q and r are integers. **Therefore the condition for diffraction is that the vector $(\boldsymbol{S} - \boldsymbol{S_o})/\boldsymbol{\lambda}$ ends on a point in the reciprocal lattice** or that

$$(\boldsymbol{S} - \boldsymbol{S_o})/\lambda = \boldsymbol{H} = h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3} \qquad (3.6)$$

Where $h, k\ and\ l$ are now restricted to integral values.

Both the Laue equations and Bragg's law can be derived from the above equation. Laue equations are obtained by forming the dot product of each side of the equation and the three crystal-lattice vectors $\boldsymbol{a_1},\ \boldsymbol{a_2},\ \boldsymbol{a_3}$ succesively. For example,

$$\boldsymbol{a_1}.(\boldsymbol{S} - \boldsymbol{S_0}/\lambda) = \boldsymbol{a_1}.(h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3})$$

$$= h$$

Thus,

$$\boldsymbol{a_1}.(\boldsymbol{S} - \boldsymbol{S_o}) = h\lambda \qquad (3.7)$$

Similarly

$$\boldsymbol{a_2}.(\boldsymbol{S} - \boldsymbol{S_o}) = k\lambda \qquad (3.8)$$

$$a_3.(\boldsymbol{S}-\boldsymbol{S_o}) = l\lambda \qquad (3.9)$$

The above equations (3.7 – 3.9) are the vector forms of the equations derived by von Laue in 1912 to express the necessary conditions for diffraction. And these three equations are called **Laue Equations.** All the three Laue equations must be satisfied simultaneously for the diffraction to occur.

3.4. Bragg's Law from Laue equation

As shown in the above Fig 3.4, the vector $(\boldsymbol{S}-\boldsymbol{S_o})$ bisects the incident beam $\boldsymbol{S_o}$ and the diffracted beam $\boldsymbol{S}$. The diffracted beam $\boldsymbol{S}$ can therefore be considered as being reflected from a set of planes perpendicular to $(\boldsymbol{S}-\boldsymbol{S_o})$. In fact equation (3.6) states that $(\boldsymbol{S}-\boldsymbol{S_o})$ is parallel to **H**, which is in turn perpendicular to the planes (*hkl*). Let θ be the angle between $\boldsymbol{S}$ $(or\ \boldsymbol{S_0})$ and these planes. Then, since $\boldsymbol{S}$ *and* $\boldsymbol{S_o}$ are unit vectors,

$$(\boldsymbol{S}-\boldsymbol{S_o}) = 2sin\theta$$

Therefore

$$\frac{2sin\theta}{\lambda} = (\boldsymbol{S}\ -\boldsymbol{S_o})/\lambda\ = \boldsymbol{H} = 1/d$$

$$2dsin\theta = n\lambda \qquad (3.10)$$

3.5. Ewald's Sphere

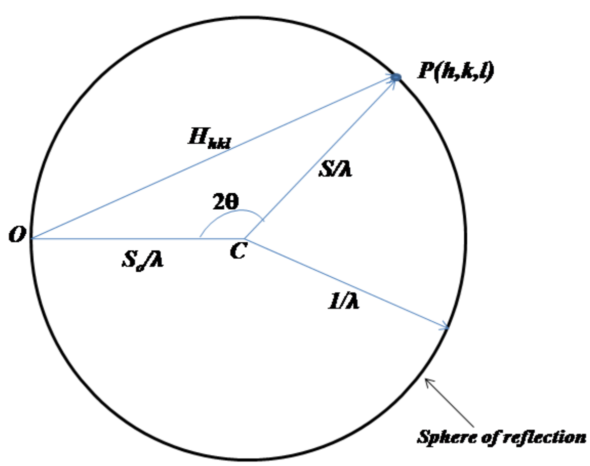

Fig 3.5

The conditions for diffraction expressed by equation (3.6) may be graphically represented by the "Ewald construction" as shown in Fig 3.5. The vector $\boldsymbol{S_o}/\lambda$ is drawn parallel to the incident beam and $1/\lambda$ in length. The terminal point $\boldsymbol{O}$ of this vector is taken as the origin of the reciprocal lattice, drawn to the same scale as the vector $\boldsymbol{S_o}/\lambda$. A sphere of radius $1/\lambda$ is drawn about C, the initial point of the incident-beam vector. Then the condition for diffraction from the (hkl) planes is that the point hkl in the reciprocal lattice (point P) touches the surface of the sphere, and the direction of the diffracted beam vector $\boldsymbol{S}/\lambda$ is found by joining $C\ to\ P$. When this condition is fulfilled, the vector **OP** equals both $\boldsymbol{H_{hkl}}$ and $(\boldsymbol{S} - \boldsymbol{S_o})/\lambda$, thus satisfying equation (3.6). Since diffraction depends on a reciprocal-lattice point touching the surface of the sphere drawn about *C*, this sphere is known as the **"sphere of reflection".**

The common methods of X-ray diffraction are differentiated by the methods used for bringing reciprocal-lattice points into contact with the surface of the sphere of reflection. The radius of the sphere may be varied by varying the incident wavelength (Laue method), or the position of the reciprocal lattice may be varied by changes in the orientation of the crystal (rotating crystal and powder diffraction).

Summary

Bragg's law can be verified either from considering the three Laue's equations and determining the intersection points of the three cones or by using Ewalds sphere construction, confirming that a reciprocal lattice point cutting the sphere of reflection will obey Bragg's law.

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