STRUCTURE OF SOLIDS

(NEP Semester V - Chapter 9)

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Crystal Diffraction and Reciprocal Lattice

- 1. Introduction
- 2. X-Ray Diffraction and Bragg's Law
- 3. Diffraction methods
- 4. Laue Method

INTRODUCTION

- Wavelengths of X-rays are of the order of 10^{-8} to 10^{-9} cm and spacing between the layers of these atoms in a crystal is in order of 10^{-8}cm, which are of the same order.
- Therefore, in 1912, German physicist Max Vor Laue suggested that the ordered arrangement of atoms in a crystal must make it to act as a three-dimensional grating.
- Thus the three dimensional crystal would be suitable for the diffraction of X-rays and diffraction pattern so obtained can give the information about the crystal structure.
- Later on, WL Bragg presented a suitable explanation of X-ray diffraction by crystal. Now x ray diffraction techniques have become a n important tool study the crystal structure.

X Ray Diffraction and Bragg's Law

- The diffraction occurs when the incident rays are reflected by atoms on the different parallel planes and these reflected rays interfere constructively and make diffraction pattern.
- By analyzing the diffraction patterns we can find out the lattice parameters, size, shape, orientation of crystal, inter planner distance etc.
- In 1913, Bragg presented a method to explain the diffraction of x ray beam.

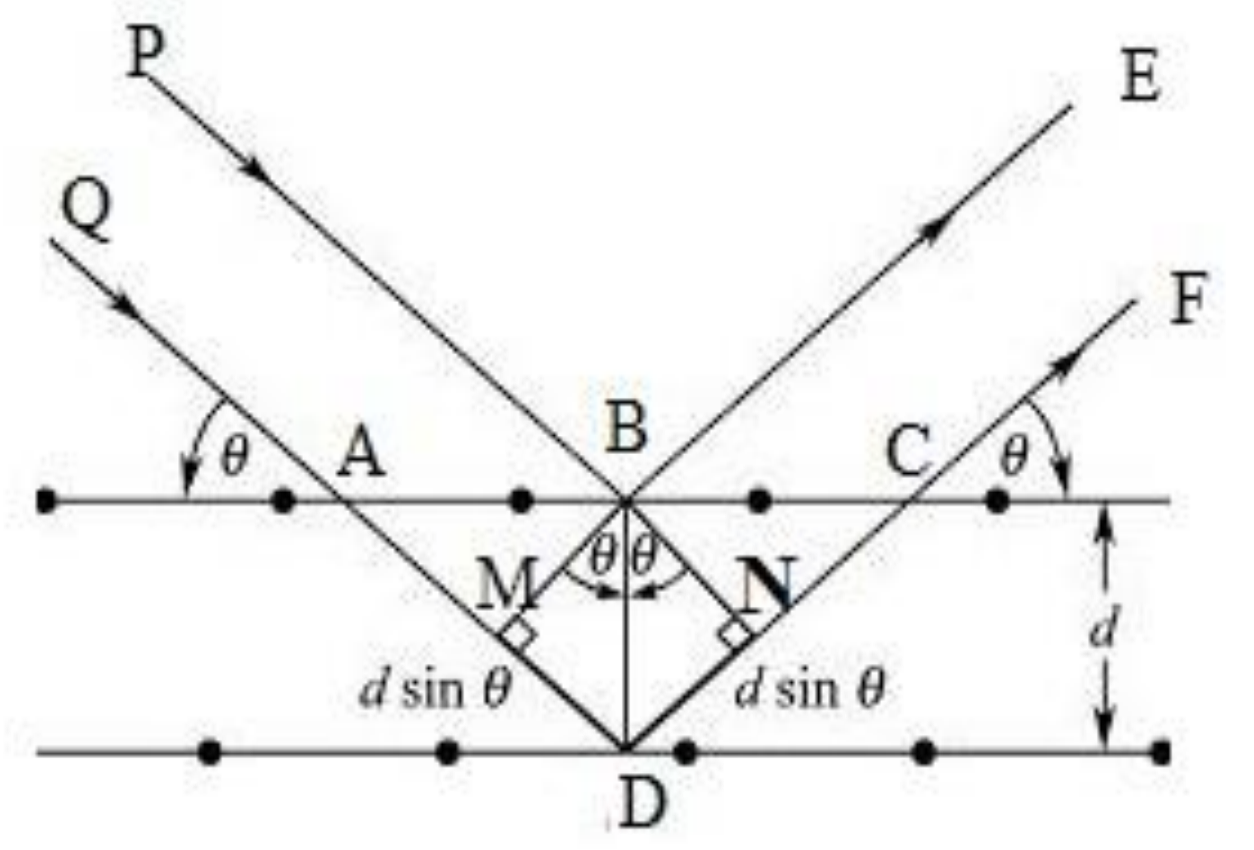


Figure2.1: Bragg's diffraction by crystal planes

- In figure the path difference between rays PBE and QDF can be given as $\Delta = MD + DN = 2MD = 2d\sin\theta$
- For constructive interference the path difference should be integral multiplication of therefore $2d\sin\theta = n\lambda$
- This is Bragg's law. The condition occurs only at certain values of λ and θ
- Thus by observing the parameters by experiment we can determine the crystal lattice spacing, size, shape, orientation and we can study the crystal structure.

Diffraction methods

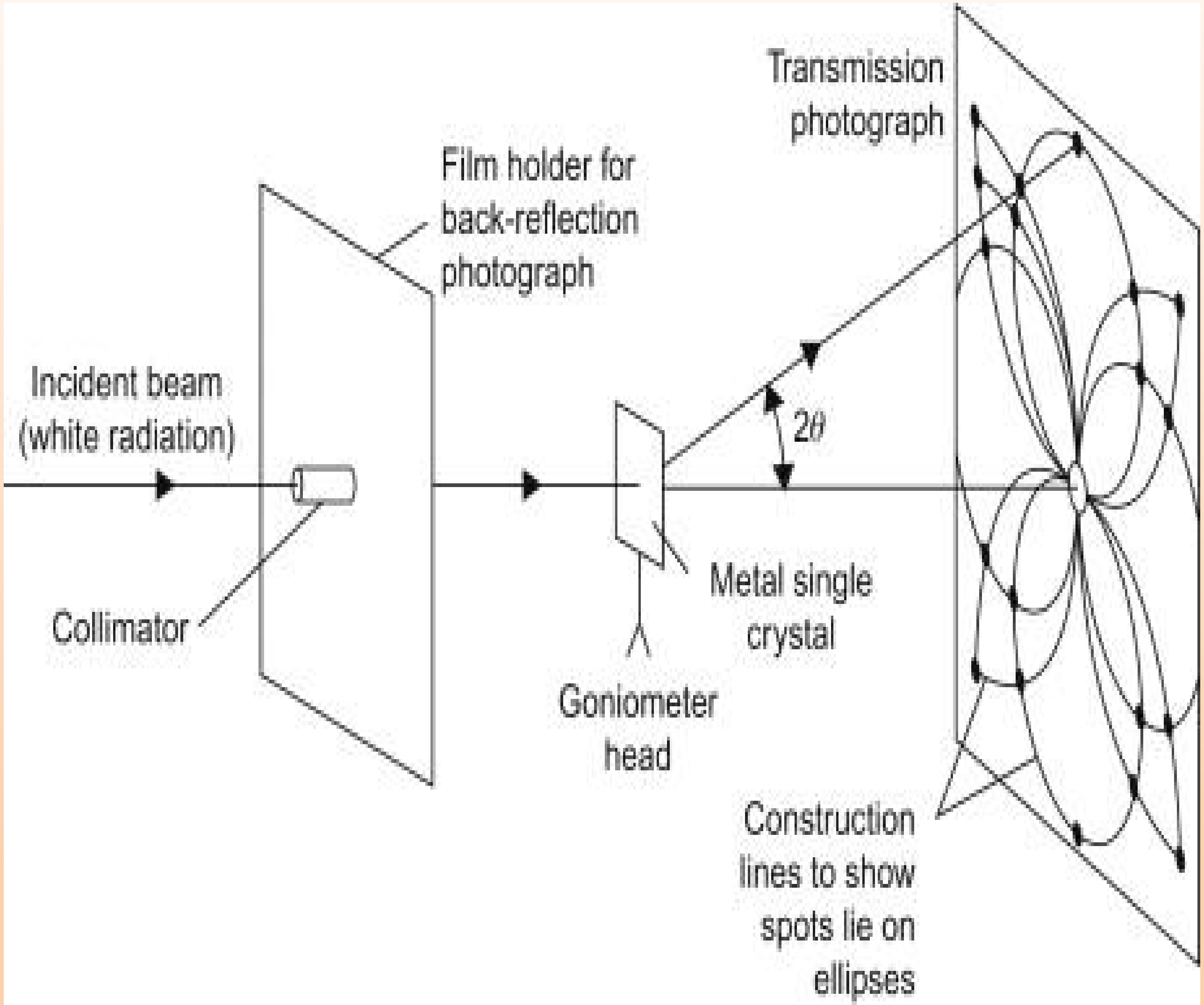
- The diffraction occurs whenever the Bragg's condition is satisfied.
- In general when monochromatic x ray beam falls on a single crystal, for arbitrary setting x rays will not produce any diffraction pattern.
- But some way if we continuously vary wavelength (λ) or diffraction angle (θ) then at a particular setting of single crystal, the Bragg's condition satisfies, and diffraction occurs.
- The ways, in which these quantities vary, there are three diffraction method as given below:

Diffraction methods

Method	Wavelength	Angle	Specimen type
Laue Method	Variable	Fixed	Single crystal
Rotating crystal method	Fixed	Varying	Single crystal
Powder method	Fixed	Variable	powder

Laue Diffraction method

- The first diffraction methods, ever used till today and it reproduces Von Laue's original experiment
- Mainly used to determine the orientations of large single crystals.
- While radiations is reflected or transmitted through a fixed single crystal, the Bragg's angle that is fixed in this particular case, for every set of planes, in the crystal and each set picks out and diffracts that particular wavelength which satisfies the Bragg's law for the particular values of dand θ
- In this particular region on to the particular film we are getting some kinds of white spots over there, which are the different diffraction picks, or maybe the spots.


Transmission
photograph
Film holder for
back-reflection
photograph
Incident beam
(white radiation)
2θ
Metal single
crystal
Collimator
Goniometer
head
Construction
lines to show
spots lie on
ellipses

Now we know that the Elastic Scattering

$$|K| = |K'|$$

$$where \quad K = \frac{S_0}{\lambda} = \text{incident wave vector}$$

$$K' = \frac{S}{\lambda} = \text{diffracted wave vector}$$

$$S_0 = \text{incoming X ray beam}$$

$$S = \text{Scattered X ray beam}$$

The Laue's theory states that for diffractions the differences in the two wave vectors must be equal to a reciprocal lattices vector.

$$K' - K = \sigma^*$$

Now from this particular case, we are going to discuss about the Ewald sphere. The Ewald sphere is a pictorial way to show the diffraction condition. We construct a sphere which is known as the Ewald constructions as shown in figure 2.3.

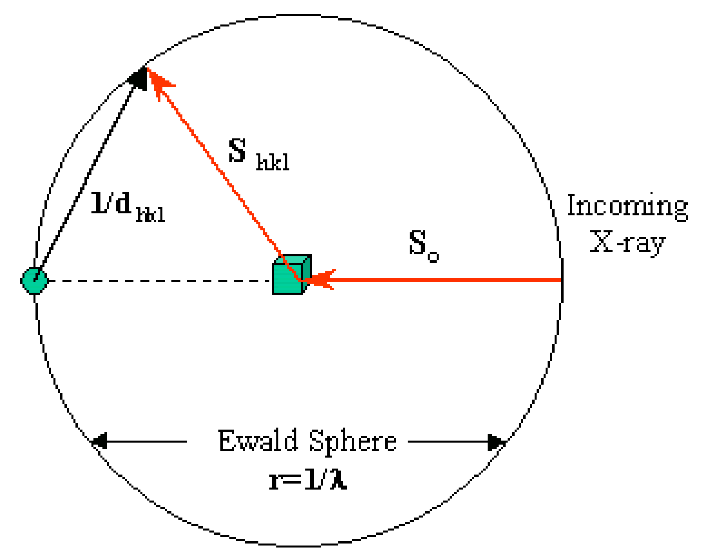


Figure 2.3: Ewald sphere

- Ewald sphere is a virtual or imaginary sphere, that sphere whose radius is 1/λ.
- The geometrical construction of Eward sphere provides the relationship between the orientations of a crystal and the directions of the beams diffracted by it.
- If the origin of reciprocal space is placed at the tip of incident beam then diffractions will occur only for those reciprocal lattice points that lie on the surface of the Ewald sphere