PROGRESSIVE EDUCATION SOCIETY'S
MODERN COLLEGE OF ENGINEERING
(An Autonomous Institute Affiliated to Savitribai Phule Pune University)
First Year B. Tech. (2024 Pattern)
Engineering Physics
Semester – I/II

Unit – 2: Diffraction

Importance of Diffraction in Engineering

Diffraction of light is an important physical phenomenon in engineering, with significant applications across various fields. Diffraction occurs when light waves encounter an obstacle or aperture and bend around it, leading to interference patterns.

Diffraction of light plays a pivotal role in various engineering disciplines, driving innovation and advancement in diverse technologies. Its significance is evident in optical communication systems, laser technology, imaging systems, optical data storage, display technology, spectroscopy, photonics, microscopy, optical sensors, and nanotechnology. Understanding diffraction enables the development of high-precision laser systems, improved imaging instruments, and enhanced optical data storage capacity. Furthermore, it informs the design of photonic devices, nano-optical structures, and advanced sensors. As research continues to push the boundaries of diffraction limits, future engineers can explore exciting prospects, such as harnessing diffraction for ultra-high-resolution imaging, developing novel optical materials, and creating more efficient optical communication networks. Studying diffraction in engineering also opens doors to emerging fields like quantum optics, metamaterials, and optogenetics. As technology advances, the importance of diffraction will only continue to grow, making its study a vital investment for the next generation of engineers seeking to revolutionize fields like telecommunications, healthcare, and energy.

Subtopics in Unit – 2

Diffraction	**2.1. Introduction to Diffraction of Light** *2.1.1. Fresnel's and Fraunhofer's Diffraction* **2.2. Diffraction at a Single Slit (Qualitative)** *2.2.1. Fraunhofer's Diffraction at a Single Slit* *2.2.1.1. Conditions for Principal Maxima Diffraction Pattern* *2.2.1.2. Conditions for Principal Minima Diffraction Pattern* *2.2.1.3. Conditions for Secondary Maxima Diffraction Pattern* *2.2.1.4. Intensity Distribution Pattern of Diffraction* **2.3. Diffraction Grating** *2.3.1. Plane Diffraction Grating* *2.3.2. Conditions for Principal Maxima* *2.3.3. Conditions for Principal Minima* **2.4. X-ray Diffraction** *2.4.1. Difference between Crystalline and Amorphous Solids* *2.4.2. Bragg's Law* *2.4.3. Analysis of XRD Spectrum for Cubic System*

Diffraction

2.1 Introduction to Diffraction of Light

When light passes through a narrow slit with a width similar to its wavelength, it spreads out well beyond the expected shadow and creates a pattern of alternating light and dark bands. This happens because light behaves like a wave, bending around the edges of openings or obstacles. This bending, which causes light to enter regions that would normally be in shadow, is called diffraction. Because of diffraction, the edges of shadows appear blurred rather than sharp, as would be expected if light traveled in straight lines. Diffraction is most noticeable when the object causing it is about the same size as the wavelength of the light. Diffraction is commonly studied using slits with narrow openings.

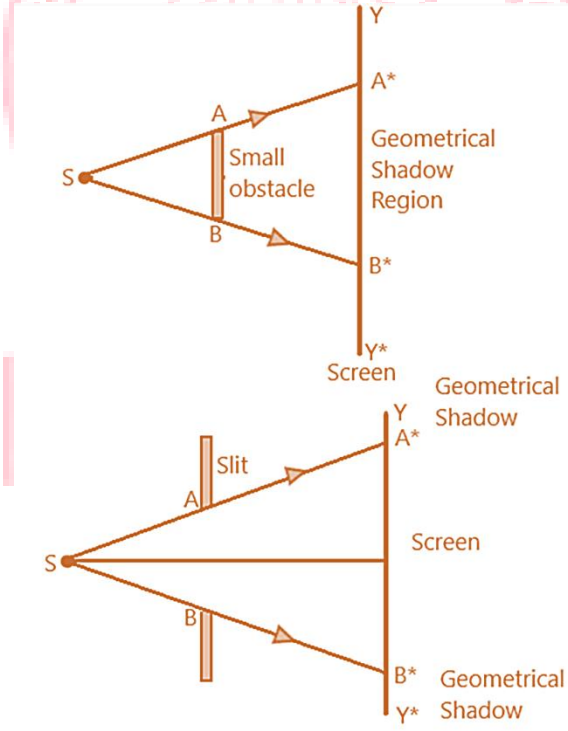

Figure 2.1. Light's straight-line travel creates sharp shadows, yet tiny obstacles reveal its wave-like bending through diffraction. This curvature defies geometric shadows. This phenomenon, known as diffraction, demonstrates light's ability to curve around edges, defying straight-line travel.[1]

Figure 2.2. Examples of diffraction of light: (a) bending of light through corners of a door, (b) light diffraction through clouds, (c) single slit diffraction.[2]

2.1.1 Fresnel and Fraunhofer Diffraction

Fresnel and Fraunhofer developed distinct diffraction theories. Fresnel Diffraction considers finite distances between source, slit, and screen, while Fraunhofer Diffraction assumes infinite distances.

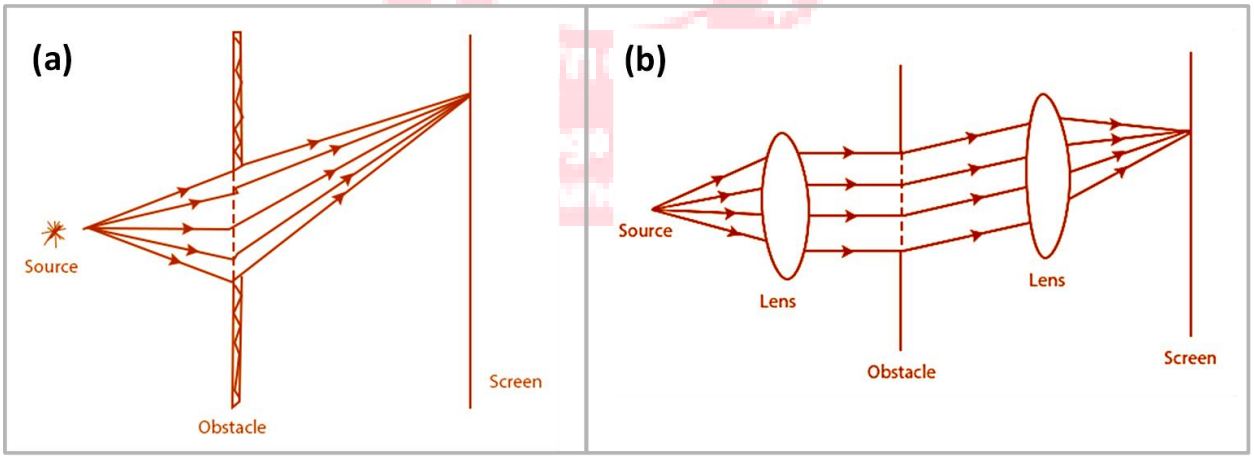

Figure 2.3. Schematic diagrams for (a) Fresnel diffraction and (b) Fraunhofer diffraction.[3]

Table 1 presents a comparative analysis of Fresnel and Fraunhofer diffraction, highlighting their primary differences.

Table 2.1. Qualitative comparison between Fresnel and Fraunhofer diffraction.

S. No.	Fresnel Diffraction	Fraunhofer Diffraction
1.	Distance of slit from source and screen is finite.	Distance of slit from source and screen is infinite.
2.	Wavefront incident on the slit is spherical or cylindrical.	Wavefront incident on the slit is plane.
3.	Wavefront incident on the screen is spherical or cylindrical.	Wavefront incident on the screen is plane.
4.	There is path difference between the rays before entering the slit which depends on the distance between the source and the slit.	There is no path difference between the rays before entering the slit.
5.	Path difference between the rays forming the diffraction pattern depends on distance of slit from source as well as the screen and the angle of diffraction. Hence, mathematical treatment is complicated.	Path difference depends only on the angle of diffraction. Hence, mathematical treatment is relatively easier.
6.	Lenses are not required to observe Fresnel diffraction in the laboratory.	Lenses are required to observe Fraunhofer diffraction in the laboratory.

2.2 Diffraction at a Single Slit

Diffraction occurs when coherent light waves are incident on an opaque barrier, B, which has an aperture of any shape. The diffraction pattern is observed on screen C, and the nature of the pattern depends on the distance between the source, the aperture, and the screen. There are three cases to consider:

1. **Very small separation**: When screen C is very close to aperture B (regardless of the distance from the source), the light travels only a short distance after passing through the aperture, with minimal spreading of the rays. In this case, diffraction effects are negligible, and the pattern on the screen is simply the geometrical shadow of the aperture.
2. **Both the source and screen are far from the aperture**: When both the source (S) and the screen (C) are far away, the incoming and outgoing wavefronts are flat, meaning the light rays

are parallel. This condition can be achieved using two converging lenses, and the type of diffraction observed in this case is called **Fraunhofer diffraction** (Figure 2.4.).

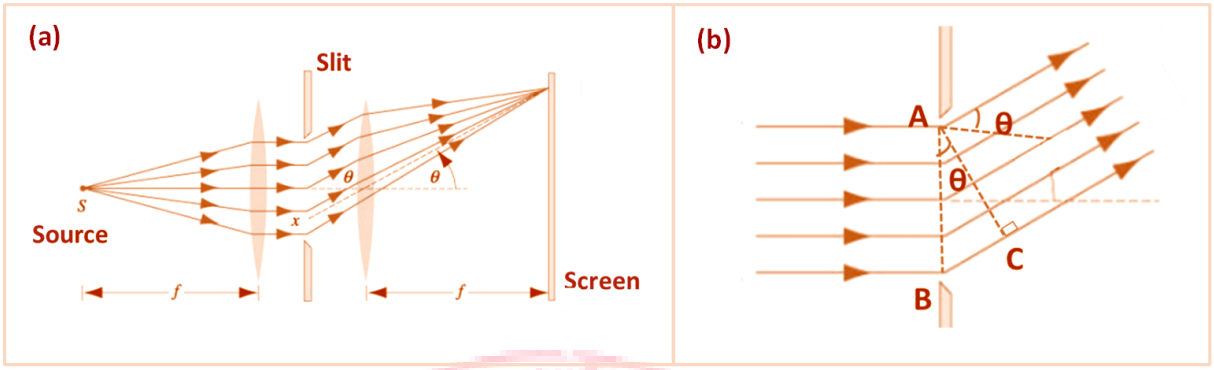

Figure 2.4. Fraunhofer diffraction.[3]

3. When **S and C are at a finite distance** from the aperture, the incident and emerging wavefronts are spherical or cylindrical. The diffraction observed in this case is known as **Fresnel diffraction** (Figure 2.5.).

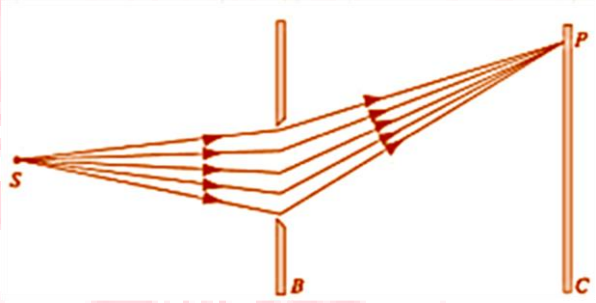

Figure 2.5. Fresnel diffraction.[3]

2.2.1 Fraunhofer Diffraction at a Single Slit (Qualitative)

To observe Fraunhofer diffraction through a single slit, consider a point source of light S positioned at the focal point of lens L_1. A second lens, L_2, is positioned beyond the slit to focus the parallel diffracted rays onto a screen located at the focal plane of the lens (Figure 2.6).

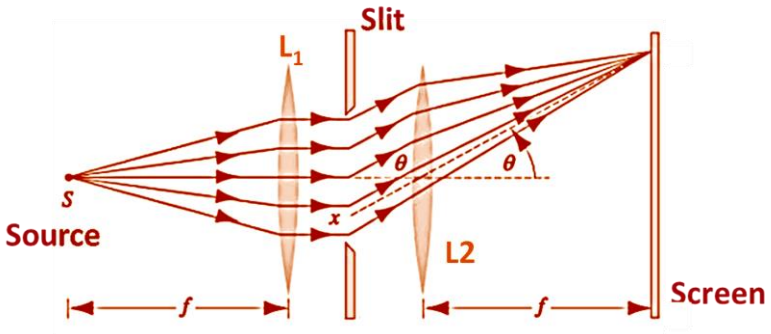

Figure 2.6. Schematic of Fraunhofer diffraction.[3]

The parallel rays from source *S* hit the single-slit AB of slit width *a*. Each point along the slit AB acts as a source of secondary wave disturbances, emitting secondary waves in all directions. After passing through lens L_2, the diffracted rays at an angle θ are brought into focus on the screen (Figure 2.7).

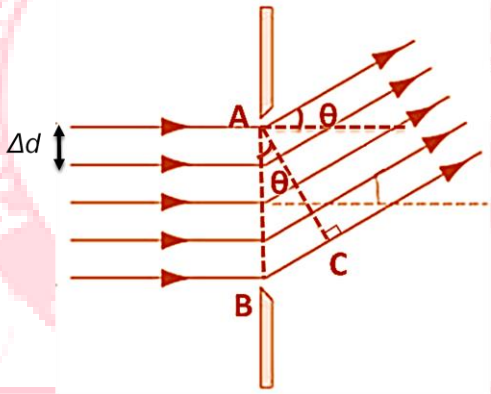

Figure 2.7. Fraunhofer diffraction through a single slit AB.[3]

The path difference between extreme rays from the slit is:

$$\Delta x = BC = AB \sin\theta = a \sin\theta$$

The *phase difference* between the rays:

$$\varphi = \frac{2\pi}{\lambda} a \sin\theta$$

The slit of width *a* is now divided into narrow strips, each with a width of *Δd* (meaning the distance between the strips is also *Δd*). These narrow strips can be thought of as sources of Huygens wavelets, and all the light from each strip arrives at a point on the screen at the same

phase. Thus, the phase difference between the waves reaching the point on the screen from two adjacent strips remains constant. Thus, the phase difference is:

$$\Delta\varphi = \frac{2\pi}{\lambda}\Delta d \sin\theta$$

To determine the resultant intensity, we represent wave disturbances as vectors and perform vector addition. N vectors of length ΔE_0 are arranged head-to-tail, with successive vectors rotated by $\Delta\varphi$, and then combined using vector addition to determine the resultant phasor amplitude (Figure 2.8).

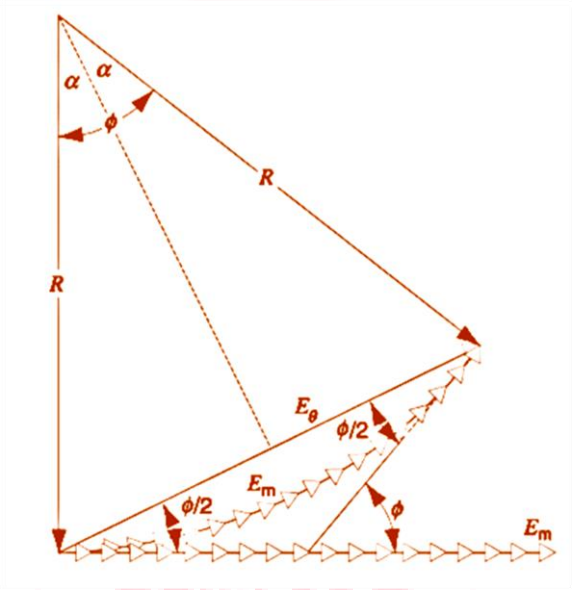

Figure 2.7. Phasor diagram to calculate the intensity in single-slit diffraction.[3]

From the diagram,

$$\alpha = \frac{\varphi}{2} = \frac{\pi}{\lambda} a \sin\theta$$

Resultant amplitude for diffraction from a single slit:

$$E_\theta = E_m \frac{\sin\alpha}{\alpha}$$

$$E_\theta^2 = E_\theta^2 \left(\frac{\sin\alpha}{\alpha}\right)^2$$

$$I_\theta = I_m \left(\frac{\sin\alpha}{\alpha}\right)^2$$

2.2.1.1. Condition for Principal Maxima

$$E_\theta = E_m \frac{\sin\alpha}{\alpha} = \frac{E_m}{\alpha}\left[\alpha - \frac{\alpha^3}{3!} + \frac{\alpha^5}{5!} - \frac{\alpha^7}{7!} + \cdots\right]$$

$$E_\theta = E_m\left[1 - \frac{\alpha^2}{3!} + \frac{\alpha^4}{5!} - \frac{\alpha^6}{7!} + \cdots\right]$$

For E_θ to be maximum, $\alpha=0$

$$\alpha = \frac{\pi}{\lambda}\, a \sin\theta = 0$$

Since, slit width, *a* cannot be zero, therefore value of α can be zero only when $\sin\theta = 0$

$$\therefore \theta = 0$$

Therefore, the principal maxima are formed along the incident direction and is also called the central maxima (Figure 2.8).

2.2.1.2. Condition for Principal Minima

For minimum intensity, $I_\theta=0$

$$\therefore\ I_m\left(\frac{\sin\alpha}{\alpha}\right)^2 = 0$$

$\alpha \neq 0$ because the expression $\left(\frac{\sin 0}{0}\right)$ is mathematically undefined and the limit would be an indeterminate form (0/0).

$$\therefore \sin\alpha = 0,\ but\ \alpha \neq 0$$

$$\therefore\ \alpha = n\pi,\quad n=\pm1, \pm2, \pm3, \ldots$$

$$\frac{\pi}{\lambda}\, a \sin\theta = n\pi$$

$$\therefore a \sin\theta = n\lambda$$

The minimum intensities are formed at angles:

$$\theta = \sin^{-1}\frac{n\lambda}{\alpha},\quad n=\pm1, \pm2, \pm3, \ldots$$

2.2.1.3. Condition for Secondary Maxima

A secondary maximum refers to the peak intensity occurring between two consecutive minimum intensities. Secondary maxima are formed under the following condition:

$$\alpha = \pm\left(n+\frac{1}{2}\right)\pi, \quad n = 1, 2, 3, \ldots$$

$$\therefore \frac{\pi}{\lambda}\, a \sin\theta = \left(n+\frac{1}{2}\right)\pi$$

$$a \sin\theta = \left(n+\frac{1}{2}\right)\lambda$$

$$\text{As, } I_\theta = I_m\left(\frac{\sin\alpha}{\alpha}\right)^2$$

$$I_\theta = I_m\left[\frac{\sin\left(n+\frac{1}{2}\right)\pi}{\left(n+\frac{1}{2}\right)\pi}\right]^2$$

$$\sin\left(n+\frac{1}{2}\right)\pi = \pm 1$$

$$\therefore \left[\sin\left(n+\frac{1}{2}\right)\pi\right]^2 = 1$$

$$\text{As, } I_\theta = \frac{1}{\left(n+\frac{1}{2}\right)^2\pi^2} I_m$$

$$\therefore \frac{I_\theta}{I_m} = \frac{1}{\left(n+\frac{1}{2}\right)^2\pi^2}, \quad n = 1, 2, 3, \ldots$$

$$\frac{I_\theta}{I_m} = 0.0450, 0.0162, 0.0083, \ldots$$

As a consequence, secondary maxima show a marked decline in intensity.

2.2.1.4. Intensity Pattern due to Single Slit

Figure 2.8 illustrates key characteristics of diffraction intensity:

- Maximum intensity occurs along the incident direction.
- Intensity drops to zero at α = ±π on either side of the central maximum.

- Alternating secondary maxima and minima emerge beyond this point.
- Secondary maxima intensity decreases sharply with distance from the center.

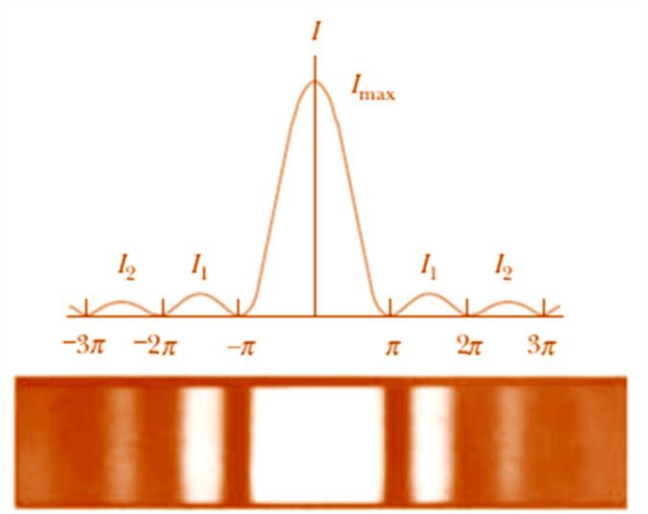

Figure 2.8. Intensity distribution in single-slit experiment.[3]

Numericals: Example and Practice Problems: Fraunhofer Single Slit Diffraction

Example: A slit of width 'a' is illuminated by white light. For what value of 'a' will the first minimum for red light (λ = 650 nm) fall at θ = 30°?

Sol: Given:

θ = 30°, n=1, λ = 650nm

Also, a sin θ = =nλ

$\therefore$ a = $\frac{n\lambda}{sin\ \theta}$

Putting the values in the above formula:

a = $\frac{1\times650\ nm}{0.5}$= 1300 nm

Problems:

2.2.1. A slit of width 'a' is illuminated by white light. For what value of 'a' does the minimum for red light (λ = 650 nm) fall at θ = 15°? (Ans: a= 2.50 µm)

2.2.2. Calculate the angular separation between the 1st order minima on either side of central maxima when the slit is 6×10^{-4} cm wide and λ=600 nm. (Ans: θ=5.74°)

2.2.3. A single slit of diffraction pattern is formed using white light. For what wavelength of light does the 2nd minimum coincide with the 3rd minimum for the wavelength 400 nm? (Ans: λ= 600 nm)

2.2.4. Find the half angular width of the central maximum in the Fraunhofer diffraction pattern of a slit of width 12×10^{-5} cm, when illuminated by light of wavelength 600 nm. (Ans: θ =30°)

2.2.5. A slit of width 2 µm is illuminated by light of wavelength 650 nm. Calculate the angle at which the 1st minimum will be observed. (Ans: θ = 18.97°)

2.2.6. A monochromatic light of wavelength 550 nm is incident normally on a slit of width 2×10^{-4} cm. Calculate the angular position of 1st and 2nd minimum. (Ans: θ_1=15.96° and θ_2=33.37°)

2.3 Diffraction Grating

A **diffraction grating** is an optical component with a pattern of closely spaced lines or grooves that diffract light into several directions. When light waves encounter the grating, they are bent, or **diffracted**, at different angles depending on the wavelength (color) of the light and the spacing of the grooves. This phenomenon causes the light to spread out into its spectrum, making diffraction gratings useful for analyzing and separating different wavelengths.

Types of diffraction grating

There are several types of diffraction gratings, each designed for different applications based on how the light interacts with the grating structure. Out of many, only two main types will be discussed here.

1. Transmission Grating: A **transmission diffraction grating** has grooves or lines etched onto a transparent material like glass. When light passes through the grating, it diffracts at different angles depending on the wavelength. These are used in Spectroscopy, wavelength separation, and optical analysis where transmitted light is needed.
2. Reflection Grating: A **reflection diffraction grating** has grooves or lines etched onto a reflective surface, typically metal or coated glass. Light is diffracted by reflecting off the surface, rather than passing through it.

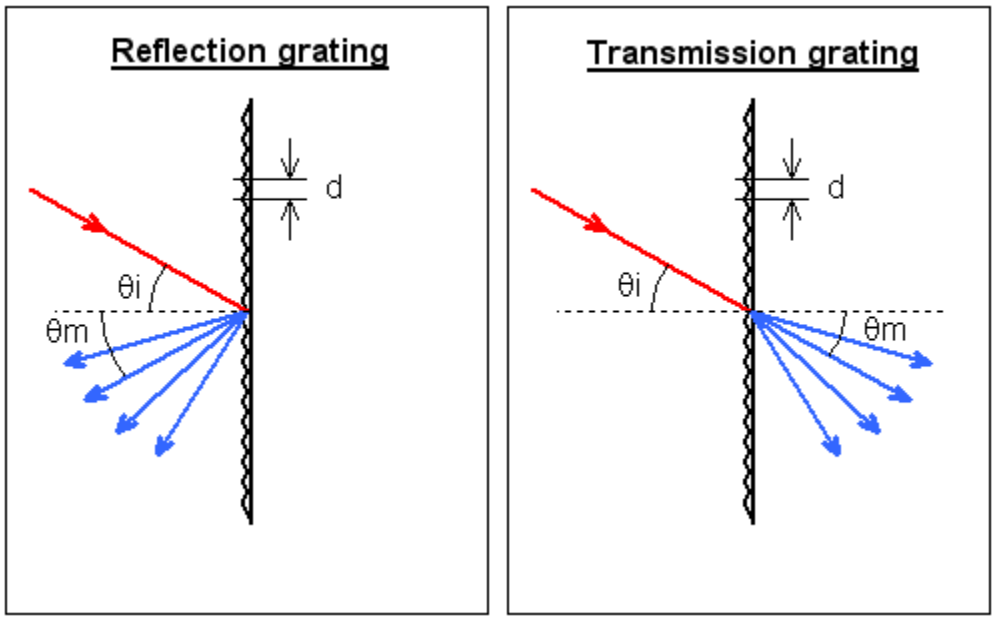

Figure 2.9. Schematic diagrams of reflection and transmission grating.[4]

2.3.1 Plane Diffraction Grating

A **plane diffraction grating** is a flat optical device consisting of a large number of equally spaced, parallel grooves or slits etched or ruled on a surface (such as glass or metal). When light passes through or reflects off this grating, it is diffracted, causing the light to spread out into its constituent wavelengths. This diffraction leads to the formation of a spectrum, making plane diffraction gratings highly useful for analyzing the composition of light.

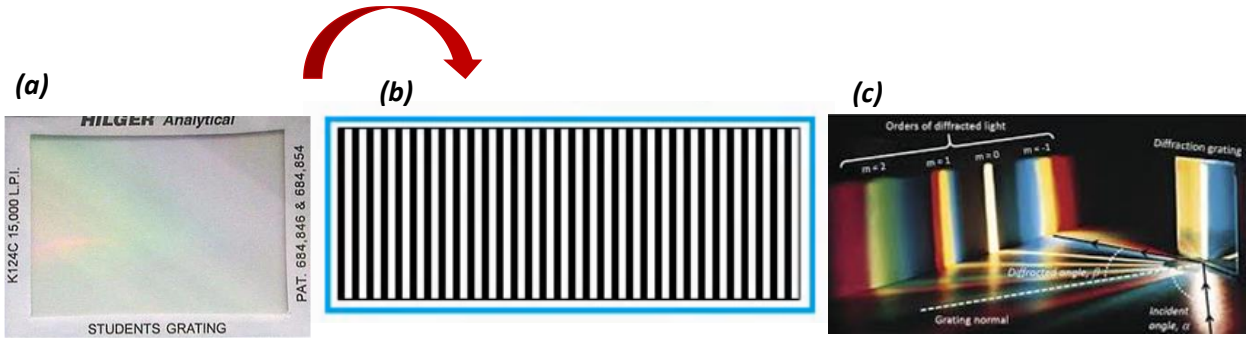

Figure 2.10. (a) A standard laboratory diffraction grating, (b) schematic of the diffraction grating having slits separated by opaque spaces, (c) diffraction pattern from a plane grating.[5]

Let,

a = width of each slit

b = width of each opaque space

N = total number of lines on the grating

So, d = a + b = width of a line (grating element)

$$\frac{1}{a+b} = number\ of\ lines\ per\ unit\ length$$

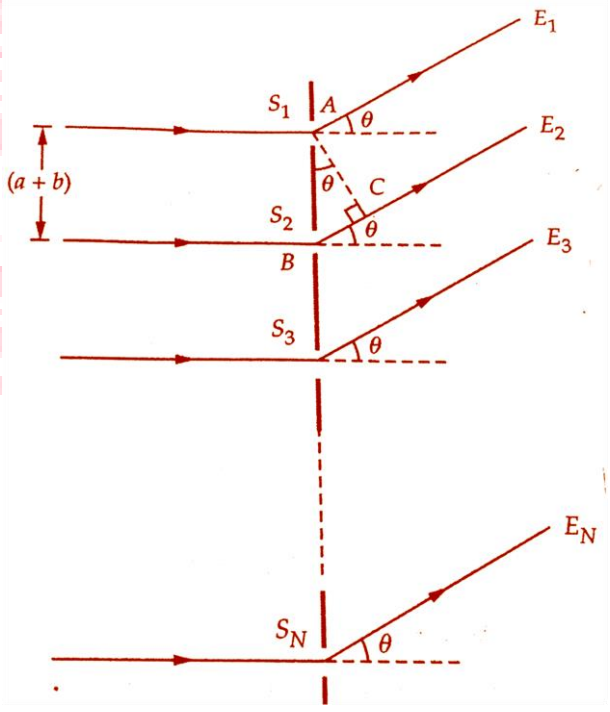

Figure 2.11. Schematic of diffraction from diffraction grating.

The resultant amplitude:

$$E_\theta = E_m\left(\frac{\sin\alpha}{\alpha}\right)\left(\frac{\sin\beta}{Sin\beta}\right), \text{ where } \beta = \frac{\pi}{\lambda}(a+b)\sin\theta$$

$$\therefore I_\theta = I_m\left(\frac{\sin\alpha}{\alpha}\right)^2\left(\frac{\sin N\beta}{Sin\beta}\right)^2$$

$I_m\left(\frac{\sin\alpha}{\alpha}\right)^2$ is the diffraction term, and $\left(\frac{\sin N\beta}{Sin\beta}\right)^2$ is the interference term due to 'N' slits.

2.3.2. Condition for Principal Maxima

The principal maxima occur when sin β = 0, corresponding to β = mπ, where m is an integer (0, ±1, ±2, ±3, …).

$$\therefore \frac{\pi}{\lambda}(a+b)\sin\theta = m\pi$$

$$\therefore (a+b)\sin\theta = \mathrm{m}\lambda$$

For β = mπ, the term $\frac{\sin N\beta}{\beta}$ becomes indeterminate.

$$\therefore I_\theta = I_m\left(\frac{\sin\alpha}{\alpha}\right)^2\left(\lim_{\beta \to m\pi}\frac{\sin N\beta}{Sin\beta}\right)^2$$

Using L'Hospital's rule:

$$I_\theta = I_m\left(\frac{\sin\alpha}{\alpha}\right)^2\left(\lim_{\beta \to m\pi}\frac{\sin N\beta}{Sin\beta}\right)^2$$

$$= I_m\left(\frac{\sin\alpha}{\alpha}\right)^2\left(\lim_{\beta \to m\pi}\frac{N\cos N\beta}{\cos\beta}\right)^2$$

For β=mπ, cos N β=cos Nmπ= ±1 and cos β= ±1

$$\therefore I_\theta = I_m\left(\frac{\sin\alpha}{\alpha}\right)^2[\pm N]2$$

$$\therefore I_\theta = N2I_m\left(\frac{\sin\alpha}{\alpha}\right)^2$$

$$\therefore I_\theta = N^2 \times \text{Intensity due to a single slit}$$

2.3.3. Condition for Principal Minima

For minimum intensity, I_θ=0

$$\therefore \frac{\sin N\beta}{\beta} = 0$$

$$\therefore \sin N\beta = 0, \ but \ \sin\beta \neq 0$$

∴ Nβ = nπ, but β≠l π where n and l are integers.

$$\therefore \beta = \frac{n\pi}{N}$$, where n/N must not be an integer.

∴ n= 1, 2, 3,…. (N-1), (N+1), (N+2), ….(2N-1), (2N+1),

or, n≠0, N, 2N,…. as these values of n give principal maxima.

As, $\beta = \frac{\pi}{\lambda}(a+b)\sin\theta$

$$\frac{\pi}{\lambda}(a+b)\sin\theta = \frac{n}{N}\pi$$

$$\therefore (a+b)\sin\theta = \frac{n}{N}\lambda$$

Where, n = 1, 2, 3, …., (N-1), (N+1), (N+2), …, (2N-1), (2N+1),…

Therefore, there are (N-1) minimum intensities between any two adjacent principal maxima.

Numericals: Example and Practice Problems: Diffraction Grating

Example: In a plane transmission grating, the angle of diffraction for the second order principal maximum for the wavelength 5×10^{-5} cm is 30°. Calculate the number of lines/cm of the grating surface.

Sol: Given:

m =2, θ = 30°, n=1, λ = 5×10^{-5} cm

Also, (a+b) sin θ = mλ

$\therefore$ a+b = $\frac{m\lambda}{sin\ \theta}$= 2×10^{-4} cm

Number of lines/cm = $\frac{1}{a+b}$ = 5000

So, there are 5000 lines/cm.

Problems:

2.3.1. What is the longest wavelength that can be observed in the 3rd order for a transmission grating having 7000 lines/cm? Assume normal incidence. (Ans: 476.2 nm)

2.3.2. Monochromatic light of wavelength 656 nm falls normally on a grating that is 2 cm wide. The 1st order spectrum is produced at an angle of 16° 12' from the normal. Calculate the total number of lines on the grating. (Ans: total number of lines=8506)

2.3.3. Monochromatic light from laser of wavelength 623.8 nm is incident normally on a diffraction grating containing 6000 lines/cm. Find the angles at which the 1st and 2nd order maximum are obtained. (Ans: θ=21.98° (for m=1), θ=48.47° (for m=2))

2.4 X-ray Diffraction

X-ray Diffraction (XRD) is a versatile, non-destructive analytical technique that has transformed the fields of materials science, structural analysis, and engineering. By leveraging the unique properties of X-rays, XRD enables researchers and engineers to probe the atomic and molecular structure of materials, uncovering critical information about their composition, crystallography, defects, and mechanical properties. This insight is invaluable for optimizing material performance, reliability, and safety in various engineering applications. In aerospace engineering, XRD informs the development of lightweight, high-strength alloys.

The discovery of X-rays by Wilhelm Conrad Röntgen in 1895 laid the foundation for XRD. Röntgen's pioneering work led to the identification of X-rays as electromagnetic radiation with wavelengths shorter than visible light. This breakthrough paved the way for Max von Laue's groundbreaking experiment in 1912, where he observed diffraction patterns from X-rays scattered by crystals.

The principle of XRD relies on the diffraction of X-rays by the atomic lattice of a crystalline material. X-rays with wavelengths typically ranging from 0.7 to 2.3 Å (Cu Kα: 1.54 Å, Mo Kα: 0.71 Å) interact with electrons in the material's atomic lattice, resulting in constructive interference and diffraction. The diffraction pattern depends on the material's crystal structure, lattice parameters (a, b, c, α, β, γ), and atomic positions.

Bragg's Law, formulated by William Henry Bragg and William Lawrence Bragg in 1913, describes the relationship between the interplanar spacing (d), angle of incidence (θ), and wavelength (λ): $2d\sin(\theta) = n\lambda$. This fundamental equation forms the basis of XRD data analysis. Modern diffractometers employ θ-2θ geometry (Figure 2.12(b)), where the detector moves 2θ while the sample moves θ.

XRD instrumentation (Figure 2.12(a)) consists of an X-ray tube (Cu, Mo, or Cr anodes), monochromator, diffractometer, and detector (scintillation counter, proportional counter, or semiconductor detector). Data analysis involves identifying peak positions (2θ angle) corresponding to d-spacings, peak intensities related to material structure and composition, and pattern matching to identify phases and crystal structures.

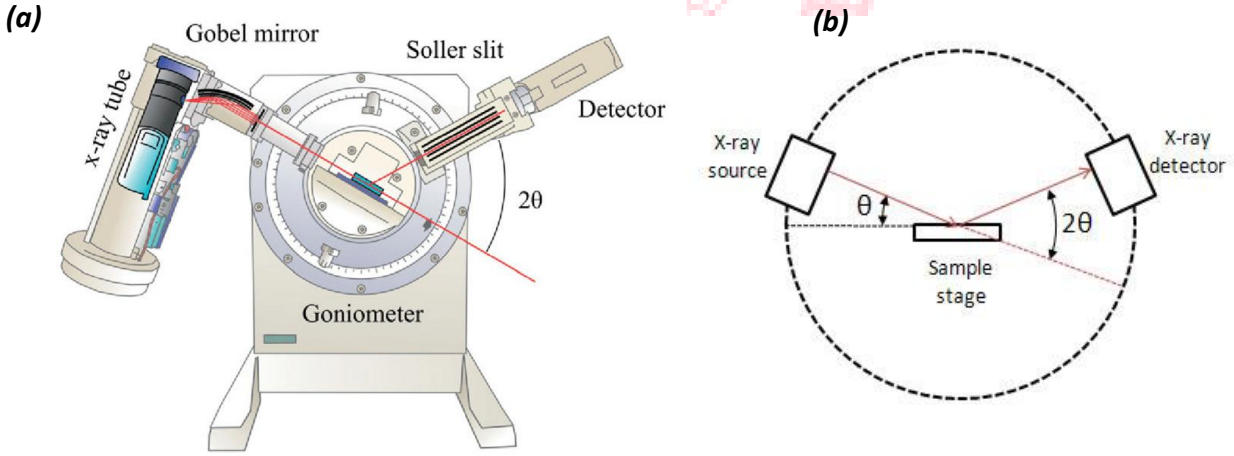

Figure 2.12. (a) A typical schematic of an XRD instrument, (b) theta-2theta geometry.[7]

2.4.1. Crystalline and Amorphous Solids

Crystalline solids are materials with a highly ordered, three-dimensional atomic arrangement, characterized by a repeating pattern of atoms or molecules.

Amorphous solids lack long-range order, with atoms or molecules arranged randomly, and lacking a repeating pattern.

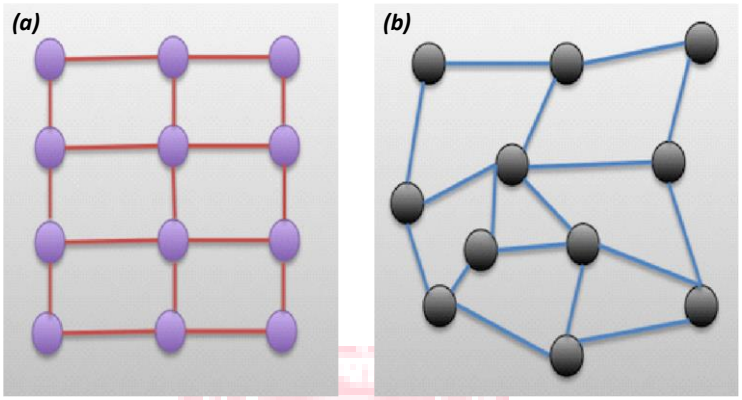

Figure 2.13. Schematic of the atomic arrangement in (a) crystalline solid and (b) amorphous solid.[8]

A comprehensive comparison between the two is presented in Table 2.

Table 2. A comprehensive comparison between a crystalline and amorphous solid.

	Crystalline Solids	Amorphous Solids
1.	Have definite and regular geometrical shapes.	Highly irregular in shape.
2.	Have a long range of orders, that's why called ordered or true solids.	Have a short range of order, that's why called disordered or pseudo solids.
3.	Have a sharp melting point.	Do not have a sharp melting point.
4.	Crystalline solids have definite heat of fusion.	Amorphous solids do not have definite heat of fusion.
5.	Highly rigid and totally incompressible.	Like crystalline solids, they are rigid too but can be compressed.
6.	When cut, they give clean and sharp cleavage.	When cut, they do not give clean and sharp cleavage.
7.	Anisotropic and symmetrical in nature.	Isotropic and unsymmetrical in nature.
8.	Examples: table salt, diamond, etc.	Examples: cotton, glass, thin-film lubricants, etc.

2.4.2. Bragg's Law

Bragg's Law is a fundamental concept in physics that describes the diffraction of waves by a crystal lattice. It explains how waves interact with the atoms in a crystal, leading to constructive

interference and diffraction. It is named after William Henry Bragg and William Lawrence Bragg, who first proposed it in 1913.

Bragg's Law states that when the X-ray is incident onto a crystal surface, its angle of incidence, θ, will reflect with the same angle of scattering, θ. And, when the path difference, d is equal to a whole number, n, of wavelength, λ, constructive interference will occur.[9]

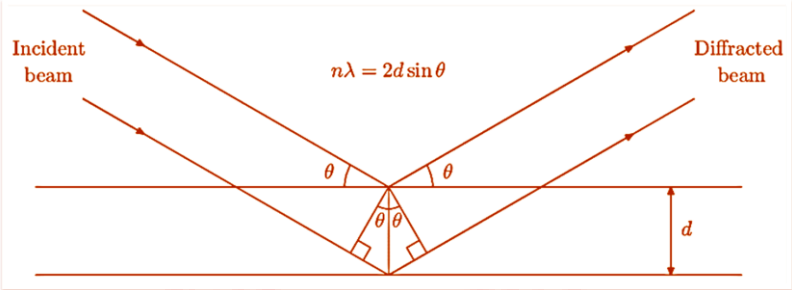

Figure 2.14. Illustration of Bragg's Law.

Bragg's Law Equation:

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

Variables:

1. d: Interplanar spacing (distance between atomic planes)
2. θ: Angle of incidence (angle between incoming wave and crystal plane)
3. n: Integer (1, 2, 3, ...) representing the order of diffraction
4. λ: Wavelength of the x-ray beam

The crystals tend to behave as reflection-type diffraction gratings due to their periodic atomic structure, comprising parallel atomic planes separated by regular distances. This acts as a three-dimensional array of scattering centres, unlike one-dimensional optical gratings. Crystals diffract x-rays similarly to how optical gratings diffract light. When x-rays hit the crystal, it scatters off (reflects) the atomic planes at the same angle, creating a pattern (diffraction phenomenon). Since x-rays short wavelengths (1-100 Å) are comparable to crystal atomic distances, it enables the process of diffraction. This diffraction pattern follows Bragg's Law, which predicts the angles at

which the radiation will scatter. The resulting diffraction pattern reveals information about the crystal structure, including its symmetry and defects.

Numericals: Example and Practice Problems: Bragg's Law

Example: **A crystal has a spacing d of 2.5 A˚. If the first-order diffraction (n=1) occurs at an angle (θ) of 30∘, what is the wavelength (λ) of the X-rays?**

Sol: **Given:**

θ = 30°, n=1, d=2.5 Å

According to Bragg's Law:

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

$$\therefore 1 \times \lambda = 2 \times (2.5\times10^{-10}\ m) \times \sin(30°)$$

$$\lambda = 2 \times (2.5\times10^{-10}\ m) \times 0.5$$

$$\lambda = 2.5\times10^{-10}\ m = 0.25\ nm$$

Problems:

2.4.1. A crystal has a spacing d of 3.5 Å. If the first-order diffraction (n=1) occurs at an angle θ of 60°, what is the wavelength λ of the X-rays? (Ans: λ = 6.06 Å)

2.4.2. X-rays scatter from a metal crystal with spacing d=2.8 Å. If the second-order diffraction (n=2) occurs at an angle θ of 75°, what is the wavelength λ? (Ans: λ =2.704 Å)

2.4.3. A semiconductor material has a crystal spacing d of 2.5 Å. If the wavelength λ of the X-rays is 1.2 Å and n=1, what is the angle θ of diffraction? (Ans: λ =13.8°)

2.4.5. X-rays scatter from a crystal at an angle θ of 45° with wavelength λ=1.0 Å and n=1. What is the interplanar spacing d? (Ans: d = 1.41 Å)

2.4.6. A crystal has a spacing d of 2.9 Å and scatters X-rays at an angle θ of 55° with wavelength λ=1.3 Å. What is the order of diffraction n? (Ans: n = 4)

The principle of XRD based on the theory of diffraction:

The principle of X-ray Diffraction (XRD) is rooted in the theory of diffraction, which describes the bending of waves around obstacles or the spreading of waves through small openings. According to wave-particle duality, X-rays exhibit both wave-like and particle-like behaviour, and as electromagnetic waves, they interact with electrons in the atomic lattice of the material. The Huygens-Fresnel Principle explains how every point on a wavefront acts as a source of secondary spherical waves, leading to constructive and destructive interference. Bragg's Law, derived from this principle, relates interplanar spacing (d) to angle of incidence (θ) and wavelength (λ): $2d \sin(\theta) = n\lambda$. This fundamental equation forms the basis of XRD, where scattered X-rays form a diffraction pattern due to constructive interference, dependent on the crystal structure of the material, lattice parameters, and atomic positions. The mathematical formulation of XRD involves the wave equation, Helmholtz equation, and Fourier transform, which relate the diffraction pattern to the crystal structure of the material. By analyzing the diffraction pattern, researchers can determine the composition of the material, crystal symmetry, lattice parameters, and defects.

2.4.3. Analysis of XRD Spectrum for Cubic System

In cubic systems (simple cubic, body-centered cubic, and face-centered cubic), the analysis of the XRD spectrum helps identify the crystal planes, calculate lattice parameters, and assess crystallite size.

For example, let us consider sodium chloride (NaCl), which has a **face-centered cubic (FCC)** crystal structure. Analyzing its XRD spectrum helps determine important properties like lattice parameters, crystallite size, and atomic arrangement.

NaCl crystallizes in a **face-centered cubic (FCC)** structure, where the sodium (Na^+) and chloride (Cl^-) ions alternate in a 3D lattice. Each Na^+ ion is surrounded by six Cl^- ions and vice versa (Figure 2.15). The lattice constant (distance between atoms) is approximately **5.64 Å (angstroms)** for NaCl.

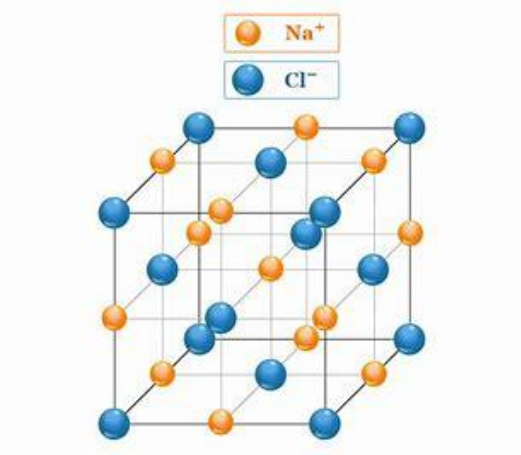

Figure 2.15. Crystal structure of NaCl.[10]

Explanation of how to analyze the XRD spectrum for NaCl:

- The XRD pattern for NaCl consists of a series of **sharp peaks** at specific angles, which correspond to the reflection from different sets of crystal planes (denoted by Miller indices hkl).

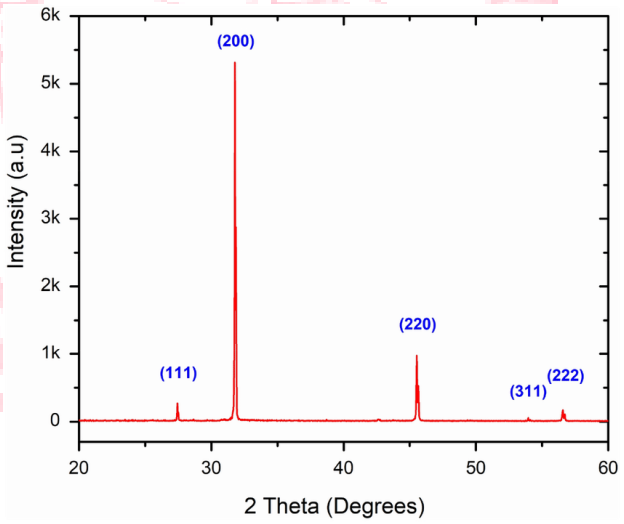

Figure 2.15. XRD spectrum of NaCl crystal.[11]

Common reflections in NaCl FCC structure are from planes such as:

- (111)
- (200)
- (220)
- (311)

Key structural parameters to analyze:

- **Position of Peaks**: The **2θ** values (angle) at which peaks occur correspond to different crystal planes. By comparing these angles with standard values from crystallographic databases (like the Joint Committee on Powder Diffraction Standards, JCPDS), we can confirm the crystal structure.
- **Intensity of Peaks**: The intensity of each peak indicates the number of atoms contributing to the reflection from that specific plane. Stronger peaks indicate more atoms aligned in that plane.
- **Miller Indices (hkl)**: Each peak corresponds to a reflection from a specific set of atomic planes, which is identified by its Miller index (hkl). The order and position of these peaks give information about the crystal symmetry.
- **Calculating Lattice Parameter**: Using Bragg's Law, we can calculate the **lattice parameter *a*** (distance between atoms) for NaCl. For an FCC structure, the relation between the plane spacing *d* and the lattice parameter a is:

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

- **Crystallite Size (Scherrer Equation)**: The broadening of XRD peaks can be used to estimate the crystallite size using the **Scherrer Equation**:

$$D = \frac{K\lambda}{\beta cos\theta}$$

Where:

- D is the crystallite size.
- K is a shape factor (usually taken as 0.9).
- λ is the X-ray wavelength.
- β is the full width at half maximum (FWHM) of the diffraction peak (in radians).
- θ is the diffraction angle.

A smaller peak width (β) indicates larger crystallite size, while broader peaks suggest smaller crystallites or more structural disorder.

Matching with Reference Data: Once the XRD spectrum is collected, the **2θ** angles of the peaks are compared to standard reference patterns (from databases like JCPDS) for NaCl. The match of the peaks' positions and intensities confirms the material's identity as NaCl.

2θ(°)	d (Å)	$(I/I_1)*100$
27.42	3.25	10
31.70	2.82	100
45.54	1.99	60
53.55	1.71	5
56.40	1.63	30
65.70	1.42	20
76.08	1.25	30
84.11	1.15	30
89.94	1.09	5

I_1: Intensity of the strongest peak

Figure 2.15. JCPDS data of XRD of NaCl single crystal.

Now, let us try to confirm the crystal structure of NaCl using the reference data shown in Figure 2.15.

Note first three strongest peaks at d1, d2, and d3

- In the present case: d1: 2.82; d2: 1.99 and d3: 1.63 Å
- Search JCPDS manual to find the d group belonging to the strongest line: between 2.84-2.80 Å
- There are 17 substances with approximately similar d2 but only 4 have d1: 2.82 Å
- Out of these, only NaCl has d3: 1.63 Å

• It is NaCl (FCC structure)

Questions:

1. Explain the term diffraction of light. What are the types of diffraction?
2. Differentiate between Fresnel and Fraunhofer diffraction.
3. Discuss qualitatively, the Fraunhofer diffraction at a single-slit.
4. The resultant amplitude of a wave when monochromatic light is diffracted from a single slit is $E_\theta = E_m(\frac{\sin\alpha}{\alpha})$. From here derive the condition for minima.
5. Calculate, approximately, the relative (with respect to central maxima) intensities of the first three maxima in the single-slit diffraction pattern.
6. Derive an expression for the intensity of the diffraction pattern in the case of single-slit, using a phasor diagram.
7. What is diffraction grating?
8. Derive conditions of maxima and minima of the diffraction pattern for a plane transmission grating, starting from the equation of resultant amplitude and intensity.
9. How would you use a diffraction grating to measure the wavelength of an unknown light source?
10. Differentiate between amorphous and crystalline solids.
11. Can an amorphous solid exhibit long-range order? Explain.
12. Compare the diffraction patterns of amorphous and crystalline solid.

Critical Thinking Questions

1. What are the limitations of using a diffraction grating for spectral analysis?

2. How does the material of the diffraction grating affect its performance?

3. Can diffraction gratings be used to focus light? Explain.

4. Can Fraunhofer gratings be used for X-ray diffraction? Explain.

5. Can a material be both amorphous and crystalline? Explain.

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