



UPSC PHYSICS OPTIONAL for CSE & IFoS

ABHI PHYSICS

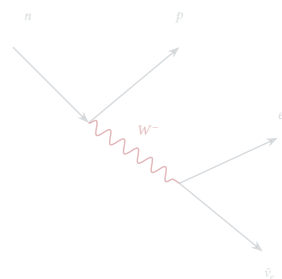
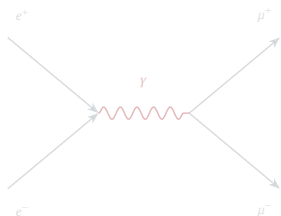
$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$$

$$[\hat{x}, \hat{p}] = i\hbar$$

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

$$E_n = -\frac{13.6}{n^2} \text{ eV}$$

PREVIOUS YEAR QUESTIONS



41 YEARS QUESTION BANK | 1986-2026

CSE + IFoS

SUBJECT

SSP and Electronic Devices

10 SOLVED QUESTIONS • CSE + IFoS

$$n \rightarrow p + e^- + \bar{\nu}_e$$

$$E^2 = p^2 c^2 + m^2 c^4$$

$$\partial_\mu j^\mu = 0$$

SUBJECT-WISE • TOPIC-WISE • SOURCE-TAGGED

For Civil Services and Indian Forest Service Examinations

Sample Preview extbar 10 Solved Questions

Question Index

No.	Question	Marks	Year	Exam	Page
1	What are the different methods used to increase the probability of exposure for the atomic planes with right orientation to X-rays in the X-rays diffraction studies?	5	2026	CSE	3
2	Explain the principle and working of the Laue's diffraction method. Comment on the origin of Laue spots and the utility of Laue's diffraction pattern.	15	2026	CSE	3
3	What is X-ray diffraction? How is an XRD pattern used to determine the crystal structure of the material?	15	2025	CSE	6
4	In powder diffraction method pattern for lead with radiation of wavelength $\lambda = 1.54 \text{ \AA}$, the (220) Bragg reflection angle is $\theta = 32^\circ$. Find the radius of the atom.	10	2025	CSE	8
5	Find the radius of the interstitial sphere which can just fit into the void at the body centre of the fcc structure coordinated by the facial atoms.	10	2025	CSE	8
6	(i) Explain the Bravais lattice and non-Bravais lattice with suitable diagram. (ii) Draw the (1 0 0), (1 1 0) and (1 1 1) planes in a cubic unit cell. (iii) Obtain the Miller indices of a plane with intercepts $a, b/2, 3c$ in a simple cubic unit cell.	10+5+5=20	2025	IFoS	9
7	The spacing between successive (100) planes in sodium chloride is $1.41 \text{ \AA}$. X-rays incident on the surface of the crystal are found to give rise to second order Bragg reflections at a glancing angle 10° . Calculate the wavelength of X-ray radiations.	10	2024	CSE	11
8	Consider the planes with indices (1 0 0) and (0 0 1); the lattice is f.c.c., and the indices refer to the conventional cubic cell. What are the indices of these planes when referred to the primitive axes : $\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y})$, $\vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z})$ and $\vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x})$?	8	2024	IFoS	11
9	Derive diffraction conditions using reciprocal lattice concept. What are these conditions known as ?	10	2023	CSE	12
10	Draw the crystal structure of CaF_2 indicating the positions of cations and anions. What are their respective coordination numbers?	10	2023	IFoS	14

CSE • 2026 • 5 MARKS

Q1. What are the different methods used to increase the probability of exposure for the atomic planes with right orientation to X-rays in the X-rays diffraction studies?

INTRODUCTION:

For diffraction from a set of parallel atomic planes of spacing d , the incident X-rays must satisfy Bragg's condition

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

where θ is the glancing angle between the incident beam and the atomic planes, λ is the X-ray wavelength, and n is the order of diffraction. Thus, for fixed d and λ , diffraction occurs only when the plane normal has the required orientation relative to the incident beam. The probability of meeting this condition can be increased by varying the wavelength, varying the crystal orientation, or simultaneously providing many randomly oriented crystallites.

SOLUTION:

The principal experimental methods are as follows.

1. Laue method: variation of wavelength

A stationary single crystal is exposed to a collimated beam of polychromatic, or "white," X-rays containing a continuous range of wavelengths. The orientations and spacings of the atomic planes remain fixed, but for a suitably oriented plane there is a greater probability that the incident spectrum contains a wavelength

$$\lambda = \frac{2d \sin \theta}{n}$$

which satisfies Bragg's law.

The diffraction spots may be recorded in transmission geometry, with the detector behind the crystal, or in back-reflection geometry, with the detector on the incident-beam side. This method is especially useful for determining crystal symmetry and orientation.

2. Rotating-crystal or oscillation method: variation of crystal orientation

A single crystal is irradiated with monochromatic X-rays and rotated continuously, or oscillated through a limited angular range, about a chosen axis. As the crystal turns, the angle θ made by each family of atomic planes with the incident beam changes. Different planes consequently pass through the required Bragg orientation

$$\theta = \sin^{-1} \left(\frac{n\lambda}{2d} \right).$$

Whenever a reciprocal-lattice point intersects the Ewald sphere, the corresponding reflected beam is recorded. Related procedures, such as the precession method, vary the crystal orientation in a controlled manner so that a larger and more conveniently arranged set of reflections is obtained.

3. Powder or Debye-Scherrer method: use of many random orientations

A finely powdered specimen contains a very large number of small crystallites whose orientations are approximately random. For any family of planes with spacing d , some crystallites will statistically have those planes at the Bragg angle θ to the incident monochromatic beam. Their diffracted rays have the same scattering angle 2θ and form a cone about the incident-beam direction. A film or position-sensitive detector intercepts this cone as rings or arcs.

The method therefore supplies the required orientations simultaneously without mechanically aligning a single crystal. It is particularly suitable for phase identification and determination of interplanar spacings.

These approaches correspond to the three quantities that can be diversified in Bragg's condition: λ is varied in the Laue method, θ is varied in rotating or oscillating-crystal methods, and a large statistical distribution of θ is supplied by the powder method. A reflection is possible only when $n\lambda \leq 2d$, since $\sin \theta \leq 1$.

CONCLUSION:

The probability of exposing atomic planes in the correct orientation is increased by:

1. using a stationary single crystal and many X-ray wavelengths in the Laue method;
2. rotating, oscillating, or precessing a single crystal in a monochromatic beam so that its plane normals successively acquire the required direction; and
3. using a powder containing numerous randomly oriented crystallites, some of which automatically have the required plane orientation.

In every case, the selected planes must be oriented at the Bragg glancing angle

$$\theta = \sin^{-1} \left(\frac{n\lambda}{2d} \right)$$

to the incident X-ray direction, equivalently with their normal making the angle $90^\circ - \theta$ with that direction.

CSE • 2026 • 15 MARKS

Q2. Explain the principle and working of the Laue's diffraction method. Comment on the origin of Laue spots and the utility of Laue's diffraction pattern.

INTRODUCTION:

Laue's method is an X-ray diffraction method in which a stationary single crystal is irradiated by a narrow beam of polychromatic, or "white," X-rays. Its principle is the coherent elastic scattering of X-rays by the periodically arranged atoms of the crystal. Although the orientation of the crystal is fixed, the continuous range of wavelengths allows different sets of lattice planes to satisfy the diffraction condition simultaneously.

Let the primitive translation vectors of the crystal be $\mathbf{a}, \mathbf{b}, \mathbf{c}$. Let $\mathbf{k}_0$ and $\mathbf{k}$ denote the incident and diffracted wave vectors, respectively, with

$$|\mathbf{k}_0| = |\mathbf{k}| = \frac{2\pi}{\lambda},$$

because X-ray diffraction is treated as elastic scattering. The scattering vector is

$$\mathbf{q} = \mathbf{k} - \mathbf{k}_0.$$

Constructive interference occurs when $\mathbf{q}$ is a reciprocal-lattice vector. The incident-beam direction is taken as fixed, and the direction of each diffracted beam is determined by the corresponding reciprocal-lattice point and the wavelength selected from the incident spectrum.

SOLUTION:

Consider identical scatterers situated at lattice points

$$\mathbf{R} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}, \quad u, v, w \in \mathbb{Z}.$$

The phase difference between waves scattered from lattice points separated by $\mathbf{R}$ is

$$\Delta\phi = (\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{R} = \mathbf{q} \cdot \mathbf{R}.$$

For constructive interference from the entire crystal, this phase difference must be an integral multiple of 2π for every lattice translation. It is therefore sufficient and necessary that

$$\mathbf{q} \cdot \mathbf{a} = 2\pi h, \quad \mathbf{q} \cdot \mathbf{b} = 2\pi k, \quad \mathbf{q} \cdot \mathbf{c} = 2\pi l,$$

where h, k, l are integers. These are the three Laue diffraction equations. Equivalently,

$$\boxed{\mathbf{k} - \mathbf{k}_0 = \mathbf{G}_{hkl}},$$

where

$$\mathbf{G}_{hkl} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

is a reciprocal-lattice vector, with the reciprocal basis defined by

$$\mathbf{a}^* \cdot \mathbf{a} = 2\pi, \quad \mathbf{a}^* \cdot \mathbf{b} = \mathbf{a}^* \cdot \mathbf{c} = 0,$$

and corresponding cyclic relations for $\mathbf{b}^*$ and $\mathbf{c}^*$.

If $(\alpha_0, \beta_0, \gamma_0)$ are the angles made by the incident beam with $\mathbf{a}, \mathbf{b}, \mathbf{c}$, and (α, β, γ) are those made by a diffracted beam, the Laue equations may also be written as

$$a(\cos \alpha - \cos \alpha_0) = h\lambda,$$

$$b(\cos \beta - \cos \beta_0) = k\lambda,$$

$$c(\cos \gamma - \cos \gamma_0) = l\lambda$$

for an orthogonal lattice with edge lengths a, b, c .

The connection with Bragg's law follows from elastic scattering. Using

$$\mathbf{k} = \mathbf{k}_0 + \mathbf{G}_{hkl}$$

and $|\mathbf{k}| = |\mathbf{k}_0|$, one obtains

$$|\mathbf{k}_0 + \mathbf{G}_{hkl}|^2 = |\mathbf{k}_0|^2,$$

so that

$$2\mathbf{k}_0 \cdot \mathbf{G}_{hkl} + |\mathbf{G}_{hkl}|^2 = 0.$$

Since $\mathbf{G}_{hkl}$ is normal to the corresponding family of lattice planes, this geometrical condition reduces to

$$\boxed{n\lambda = 2d_{hkl} \sin \theta},$$

where d_{hkl} is the interplanar spacing, θ is the glancing angle, and n is the diffraction order. Thus, the Laue equations and Bragg's law express the same condition in vector and plane descriptions, respectively.

The experimental working is as follows:

1. A beam of white X-rays, containing a continuous range of wavelengths, is produced by an X-ray tube and made narrow and approximately parallel by collimating slits.
2. A stationary single crystal is placed in the path of the collimated beam. Its orientation remains fixed throughout the exposure.
3. For a particular family of planes, d_{hkl} and θ are fixed because the crystal is stationary. From the incident continuous spectrum, only the wavelength

$$\lambda = \frac{2d_{hkl} \sin \theta}{n}$$

that lies within the available spectral range is strongly diffracted.

4. Many differently oriented plane families can select different wavelengths at the same time. Consequently, several diffracted beams emerge in different directions.

5. A photographic film or a two-dimensional X-ray detector records the intersections of these diffracted beams with the detector surface. The direct transmitted beam is normally intercepted or identified separately.

Two commonly used arrangements are:

1. In the transmission Laue method, the detector is placed behind the crystal, approximately normal to the incident beam. The forward-diffracted rays produce spots around the transmitted-beam position. This arrangement is suitable especially for relatively thin crystals.
2. In the back-reflection Laue method, the detector is placed on the incident-beam side of the crystal, with an opening through which the primary beam passes. The detector records rays diffracted through large angles. This arrangement is useful for thick or strongly absorbing specimens because the radiation need penetrate only a limited depth.

Each observed Laue spot originates from constructive interference associated with a reciprocal-lattice vector $\mathbf{G}_{hkl}$, or equivalently with a particular set of lattice planes. Since the crystal is not rotated, the spot does not arise because a plane family is mechanically brought into reflection position. Instead, that family selects from the white spectrum the wavelength that satisfies Bragg's law. Thus different spots generally correspond not only to different (hkl) plane families but also to different wavelengths.

In reciprocal-space language, the incident wave vectors of different magnitudes form a range of Ewald spheres because $|\mathbf{k}_0| = 2\pi/\lambda$ varies across the white spectrum. A reflection occurs whenever one of these spheres passes through a reciprocal-lattice point. The direction of the corresponding diffracted wave vector fixes the location of the spot on the detector.

The spots are discrete because the translational periodicity of a well-ordered crystal permits strong diffraction only at reciprocal-lattice points. Their intensities depend on the incident spectral intensity, polarization and geometrical factors, absorption, multiplicity, and especially the crystal structure factor

$$F_{hkl} = \sum_j f_j \exp[2\pi i(hx_j + ky_j + lz_j)],$$

where f_j and (x_j, y_j, z_j) are the atomic scattering factor and fractional coordinates of the j -th atom in the unit cell. A geometrically allowed spot may therefore be weak or absent when $F_{hkl} = 0$.

The Laue pattern has the following principal uses:

1. *Determination of crystal orientation:* The positions of the spots identify the directions of crys-

tallographic axes relative to the incident beam. The method is widely used to align single crystals before cutting, polishing, or carrying out other diffraction measurements.

2. *Identification of symmetry:* The symmetry of the spot pattern about the incident-beam direction reveals the corresponding rotational and mirror symmetry of the crystal orientation, subject to the diffraction symmetry and possible intensity equivalences.
3. *Testing whether a specimen is a single crystal:* A well-oriented single crystal produces an orderly array of sharp spots. Several differently oriented crystals or grains produce superposed sets of spots.
4. *Assessment of crystal quality:* Sharp, regular spots indicate good long-range order. Split, streaked, diffuse, broadened, or distorted spots can reveal mosaic structure, strain, lattice defects, bending, disorder, or imperfect crystallinity.
5. *Observation of orientation changes:* Changes in spot positions can be used to study crystal rotation, deformation, recrystallization, and related structural changes.
6. *Rapid crystallographic identification:* Comparison of the measured spot geometry with calculated or standard patterns helps identify crystallographic directions and, in suitable cases, distinguish possible crystal symmetries.

Because each spot normally involves a different and not always precisely known wavelength, an ordinary Laue photograph is less convenient for accurate determination of lattice constants or a complete crystal structure than monochromatic rotating-crystal or powder methods. Its chief strength is the rapid determination of orientation, symmetry, and crystal perfection.

CONCLUSION:

Laue's method uses a stationary single crystal and a collimated polychromatic X-ray beam. Diffraction occurs in directions satisfying

$$\mathbf{k} - \mathbf{k}_0 = \mathbf{G}_{hkl},$$

or, in direct-lattice form,

$$\mathbf{q} \cdot \mathbf{a} = 2\pi h, \quad \mathbf{q} \cdot \mathbf{b} = 2\pi k, \quad \mathbf{q} \cdot \mathbf{c} = 2\pi l.$$

For elastic scattering these conditions are equivalent to

$$n\lambda = 2d_{hkl} \sin \theta.$$

Each reciprocal-lattice point that can satisfy this condition selects an appropriate wavelength, measured in

units of length, from the white spectrum and sends a diffracted beam in a definite direction. Its intersection with the detector forms a Laue spot. The method is valid when the specimen has sufficient crystalline order, the scattering is predominantly elastic, and the required wavelength lies within the incident spectrum. The positions, symmetry, sharpness, splitting, and intensities of the spots provide rapid information about crystal orientation, symmetry, single-crystal character, strain, defects, and overall crystal quality.

CSE • 2025 • 15 MARKS

Q3. What is X-ray diffraction? How is an XRD pattern used to determine the crystal structure of the material?

INTRODUCTION:

X-ray diffraction (XRD) is the coherent elastic scattering of X-rays by the periodically arranged atoms of a crystalline material. Since X-ray wavelengths, typically of order 10^{-10} m, are comparable to interatomic spacings, waves scattered from different lattice planes interfere. Constructive interference produces diffraction peaks whose positions, intensities, and shapes contain information about the crystal structure.

Consider monochromatic radiation of wavelength λ incident on a set of parallel lattice planes separated by d_{hkl} , where (hkl) are Miller indices. Let θ be the glancing angle between the incident beam and the planes; the angle between the incident and diffracted beams is then 2θ . The discussion assumes a crystalline specimen, predominantly elastic and kinematic scattering, and an accurately known wavelength and instrumental geometry.

SOLUTION:

For rays scattered by two successive lattice planes, the extra distance travelled by the lower ray is

$$\Delta = 2d_{hkl} \sin \theta.$$

Constructive interference requires this path difference to be an integral multiple of the wavelength:

$$2d_{hkl} \sin \theta = n\lambda, \quad n = 1, 2, \dots$$

This is Bragg's law. Higher-order diffraction may equivalently be indexed as first-order diffraction from another reciprocal-lattice plane, so XRD patterns are ordinarily indexed using $n = 1$:

$$d_{hkl} = \frac{\lambda}{2 \sin \theta_{hkl}}.$$

An XRD pattern records diffracted intensity I as a function of 2θ . In a powder specimen, the crystal-

lites are randomly oriented; for every allowed family of lattice planes, some crystallites satisfy Bragg's condition. Consequently, each plane family produces a diffraction cone, detected as a peak at a definite value of 2θ .

The crystal structure is determined from the pattern as follows.

1. *Determine the interplanar spacings from peak positions.*

For every measured peak at $2\theta_i$, its Bragg angle is $\theta_i = (2\theta_i)/2$, and

$$d_i = \frac{\lambda}{2 \sin \theta_i}.$$

Thus the peak positions give a set of experimental interplanar spacings. These spacings are compared with the metric relations appropriate to possible crystal systems. For an orthogonal unit cell,

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2},$$

where a, b, c are the lattice parameters. Important special cases are

$$\text{cubic:} \quad \frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2},$$

$$\text{tetragonal:} \quad \frac{1}{d_{hkl}^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2},$$

$$\text{orthorhombic:} \quad \frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}.$$

For a cubic crystal, Bragg's law gives

$$\sin^2 \theta_{hkl} = \frac{\lambda^2}{4a^2} (h^2 + k^2 + l^2).$$

Hence the ratios of experimental $\sin^2 \theta$ values must equal ratios of the allowed integers $h^2 + k^2 + l^2$. Matching these ratios assigns Miller indices to the peaks and determines the lattice constant through

$$a = d_{hkl} \sqrt{h^2 + k^2 + l^2} = \frac{\lambda \sqrt{h^2 + k^2 + l^2}}{2 \sin \theta_{hkl}}.$$

A consistent value of a from several independently indexed peaks is an important test of the proposed indexing.

2. *Identify the Bravais lattice from systematic absences.*

Not every geometrically possible reflection has nonzero intensity. Translational symmetry

causes characteristic reflection conditions. For conventional cubic lattices,

Bravais lattice	Allowed reflections
primitive cubic (P)	all integral h, k, l ,
body-centred cubic (I)	$h + k + l$ even,
face-centred cubic (F)	h, k, l all even or all odd.

These conditions follow from the lattice structure factor. For identical atoms with atomic scattering factor f ,

$$F_{hkl} = \sum_j f e^{2\pi i(hx_j + ky_j + lz_j)},$$

where (x_j, y_j, z_j) are fractional atomic coordinates.

For example, a body-centred lattice has atoms at $(0, 0, 0)$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, so

$$F_{hkl} = f \left[1 + e^{i\pi(h+k+l)} \right].$$

Therefore $F_{hkl} = 2f$ when $h + k + l$ is even, but $F_{hkl} = 0$ when it is odd. The missing odd-sum reflections consequently identify body centring. Analogous systematic absences distinguish face centring and other translational symmetries.

3. Determine the atomic basis from relative intensities.

The integrated intensity of a reflection is, in simplified form,

$$I_{hkl} \propto m_{hkl} L_{hkl} P_{hkl} |F_{hkl}|^2 e^{-2M_{hkl}},$$

where m_{hkl} is the multiplicity, $L_{hkl} P_{hkl}$ represents geometrical and polarization corrections, and $e^{-2M_{hkl}}$ is the thermal factor. For a basis containing different atoms,

$$F_{hkl} = \sum_j f_j e^{2\pi i(hx_j + ky_j + lz_j)}.$$

The factors f_j depend on the atomic species and scattering angle. Because the measured intensity is governed by $|F_{hkl}|^2$, different arrangements of atoms within the same unit cell produce different relative peak intensities even when their peak positions are identical. Trial structural models are therefore used to calculate intensities, which are compared with the observed values to infer the atomic species, fractional coordinates, site occupancies, and thermal displacements.

4. Refine and validate the structural model.

After determining a probable crystal system, Bravais lattice, unit-cell dimensions, and atomic basis, a calculated complete pattern is

fitted to the observed pattern. In Rietveld refinement, structural and profile parameters are varied simultaneously to minimize a weighted residual such as

$$S = \sum_i w_i [I_i^{\text{obs}} - I_i^{\text{calc}}]^2.$$

Agreement must extend over the entire pattern: peak positions test the unit-cell metric, systematic absences test lattice symmetry, relative intensities test the atomic basis, and peak profiles provide information about crystallite size, microstrain, defects, and instrumental broadening. Unindexed peaks may indicate an incorrect model or the presence of additional crystalline phases.

The diffraction condition also has a reciprocal-space interpretation. If $\mathbf{k}_0$ and $\mathbf{k}$ are the incident and elastically scattered wavevectors, with

$$|\mathbf{k}_0| = |\mathbf{k}| = \frac{2\pi}{\lambda},$$

then diffraction occurs when the scattering vector equals a reciprocal-lattice vector:

$$\mathbf{k} - \mathbf{k}_0 = \mathbf{G}_{hkl}.$$

This form makes clear that peak positions determine the reciprocal lattice, whereas intensities determine how atoms are distributed within the corresponding real-space unit cell.

XRD has intrinsic limitations. Since an ordinary diffraction measurement records $|F_{hkl}|^2$ rather than the phase of F_{hkl} , atomic positions cannot generally be obtained by direct inversion without additional structural constraints or phase-determination methods. Furthermore, amorphous materials produce broad diffuse features rather than a set of sharp Bragg peaks, and preferred orientation, overlapping peaks, multiphase samples, and light elements can complicate structure determination.

CONCLUSION:

X-ray diffraction is the coherent elastic scattering of X-rays by a periodic crystal lattice, with diffraction maxima satisfying

$$2d_{hkl} \sin \theta = n\lambda.$$

An XRD pattern determines crystal structure through complementary information: peak positions yield d_{hkl} , lattice parameters, and the crystal system; systematic absences identify translational symmetry and the Bravais lattice; relative integrated intensities, through

$$I_{hkl} \propto |F_{hkl}|^2,$$

determine the atomic basis; and whole-pattern refinement tests and improves the complete structural

model. The inferred structure is reliable when one indexed unit cell consistently accounts for the observed peak positions, extinction rules, and corrected intensities, subject to the assumptions of adequate crystallinity, known wavelength, suitable diffraction geometry, and proper allowance for instrumental and specimen effects.

CSE • 2025 • 10 MARKS

Q4. In powder diffraction method pattern for lead with radiation of wavelength $\lambda = 1.54 \text{ \AA}$, the (220) Bragg reflection angle is $\theta = 32^\circ$. Find the radius of the atom.

INTRODUCTION:

Lead crystallizes in the face-centred cubic (FCC) structure. We assume the conventional hard-sphere model in which neighbouring atoms touch along a face diagonal. The indexed (220) powder line is taken as a first-order Bragg reflection, and the given θ is the Bragg angle between the incident beam and the reflecting lattice planes.

Let a be the cubic lattice parameter, d_{220} the spacing of the (220) planes, and R the atomic radius. Bragg's law and the interplanar-spacing relation for a cubic crystal will be used to determine a , after which the FCC contact geometry gives R .

SOLUTION:

For first-order diffraction, Bragg's law is

$$\lambda = 2d_{220} \sin \theta.$$

Hence,

$$d_{220} = \frac{\lambda}{2 \sin \theta}.$$

For a cubic crystal,

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}.$$

Therefore, for the (220) planes,

$$d_{220} = \frac{a}{\sqrt{2^2 + 2^2 + 0^2}} = \frac{a}{\sqrt{8}} = \frac{a}{2\sqrt{2}}.$$

Substitution in Bragg's law gives

$$\lambda = 2 \left(\frac{a}{2\sqrt{2}} \right) \sin \theta = \frac{a \sin \theta}{\sqrt{2}},$$

so that

$$a = \frac{\sqrt{2}\lambda}{\sin \theta}.$$

In an FCC unit cell, atoms touch along a face diagonal. The face diagonal has length $a\sqrt{2}$ and contains four atomic radii:

$$4R = a\sqrt{2}.$$

Thus,

$$R = \frac{a\sqrt{2}}{4} = \frac{a}{2\sqrt{2}}.$$

Using the expression for a ,

$$R = \frac{1}{2\sqrt{2}} \left(\frac{\sqrt{2}\lambda}{\sin \theta} \right) = \frac{\lambda}{2 \sin \theta}.$$

Equivalently, for FCC lead, $R = d_{220}$.

Substituting the given values,

$$R = \frac{1.54 \text{ \AA}}{2 \sin 32^\circ} = \frac{1.54 \text{ \AA}}{2(0.5299)} = \frac{1.54 \text{ \AA}}{1.0598} \approx 1.45 \text{ \AA}.$$

In SI units,

$$R \approx 1.45 \times 10^{-10} \text{ m}.$$

The corresponding lattice parameter is

$$a = 2\sqrt{2} R \approx 2\sqrt{2}(1.45 \text{ \AA}) \approx 4.11 \text{ \AA},$$

which is physically consistent with an FCC metal having an atomic diameter $2R \approx 2.90 \text{ \AA}$.

CONCLUSION:

The radius of a lead atom, treating FCC atoms as touching hard spheres, is

$$R \approx 1.45 \text{ \AA} = 1.45 \times 10^{-10} \text{ m}.$$

CSE • 2025 • 10 MARKS

Q5. Find the radius of the interstitial sphere which can just fit into the void at the body centre of the fcc structure coordinated by the facial atoms.

INTRODUCTION:

Let the radius of each atom forming the ideal face-centred cubic structure be R , the cube-edge length be a , and the radius of the interstitial sphere be r . The atoms are treated as identical rigid spheres. In an fcc structure, neighbouring atoms touch along each face diagonal.

The void at the body centre is surrounded by the six face-centred atoms, one on each face of the cube, and is therefore an octahedral void of coordination number 6. Taking the body centre and a face centre on a common Cartesian axis, the distance between them is $a/2$. For a sphere that just fits into the void, it must touch each of these six atoms.

SOLUTION:

The length of a face diagonal of the cubic unit cell is

$$\sqrt{a^2 + a^2} = \sqrt{2}a.$$

Along this diagonal, the two corner atoms and the intervening face-centred atom are in contact. Hence the face diagonal equals four atomic radii:

$$\sqrt{2}a = 4R.$$

Therefore,

$$a = \frac{4R}{\sqrt{2}} = 2\sqrt{2}R.$$

The distance from the body centre,

$$\left(\frac{a}{2}, \frac{a}{2}, \frac{a}{2}\right),$$

to the centre of the atom on, for example, the face $x = 0$,

$$\left(0, \frac{a}{2}, \frac{a}{2}\right),$$

is

$$d = \sqrt{\left(\frac{a}{2}\right)^2 + 0^2 + 0^2} = \frac{a}{2}.$$

When the interstitial sphere just fits, it touches the face-centred atom externally. Thus,

$$R + r = \frac{a}{2}.$$

Using $a = 2\sqrt{2}R$,

$$R + r = \frac{2\sqrt{2}R}{2} = \sqrt{2}R,$$

so that

$$r = (\sqrt{2} - 1)R.$$

Numerically,

$$\frac{r}{R} = \sqrt{2} - 1 = 1.4142 - 1 \approx 0.414.$$

The corner atoms are farther from the body centre than the facial atoms: their centre-to-centre distance is

$$\frac{\sqrt{3}a}{2} = \sqrt{6}R,$$

which exceeds $R + r = \sqrt{2}R$. Hence the six face-centred atoms, rather than the corner atoms, determine the limiting size of the interstitial sphere.

CONCLUSION:

The body-centred void in an ideal fcc structure is an octahedral void coordinated by six face-centred atoms. The radius of the largest interstitial sphere that can just fit into it is

$$r = (\sqrt{2} - 1)R \approx 0.414R,$$

where R is the radius of an atom of the fcc lattice. Thus, the interstitial sphere can have at most approximately 41.4% of the host-atom radius.

IFoS • 2025 • 10+5+5=20 MARKS

Q6. (i) Explain the Bravais lattice and non-Bravais lattice with suitable diagram. (ii) Draw the (1 0 0), (1 1 0) and (1 1 1) planes in a cubic unit cell. (iii) Obtain the Miller indices of a plane with intercepts a , $b/2$, $3c$ in a simple cubic unit cell.

INTRODUCTION:

A Bravais lattice is an infinite periodic array of geometrically equivalent points generated by integral translations

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3, \quad n_1, n_2, n_3 \in \mathbb{Z},$$

where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are primitive translation vectors. Every Bravais-lattice point therefore has the same surroundings and can be carried into every other lattice point by a lattice translation.

The expression “non-Bravais lattice” is conventionally used for a periodic atomic arrangement whose sites cannot all be generated from one site by translations alone. More precisely, it is a crystal structure consisting of a Bravais lattice supplied with a basis of two or more inequivalent sites.

For the crystallographic parts, take a right-handed Cartesian frame with the origin at a corner of the unit cell and the positive x , y , and z axes along the crystallographic axes of lengths a , b , and c , respectively. A plane with intercepts pa , qb , and rc has Miller indices proportional to

$$\left(\frac{1}{p}, \frac{1}{q}, \frac{1}{r}\right),$$

after clearing fractions and reducing to the smallest relatively prime integers. An infinite intercept has reciprocal zero. For the cubic cell in part (ii), $a = b = c$, and the plane (hkl) may be represented by

$$h\frac{x}{a} + k\frac{y}{a} + l\frac{z}{a} = 1.$$

SOLUTION:

- (i) For a Bravais lattice, translation by any lattice vector $\mathbf{R}$ leaves the complete array invariant. Thus, if $\mathbf{R}_1$ and $\mathbf{R}_2$ are any two lattice points, then

$$\mathbf{R}_2 - \mathbf{R}_1$$

is a lattice translation, and the local environment at $\mathbf{R}_1$ is identical to that at $\mathbf{R}_2$ with the same orientation.

A square array containing one identical point per primitive cell is a two-dimensional example:

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2, \quad n_1, n_2 \in \mathbb{Z}.$$

In contrast, suppose every square Bravais-lattice point carries a two-site basis

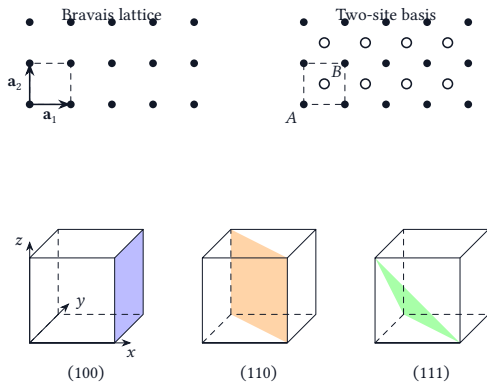
$$\boldsymbol{\tau}_A = \mathbf{0}, \quad \boldsymbol{\tau}_B = \frac{\mathbf{a}_1 + \mathbf{a}_2}{2},$$

where A and B denote inequivalent atoms or sites. The positions are then

$$\mathbf{r}_{n,s} = \mathbf{R}_n + \boldsymbol{\tau}_s, \quad s = A, B.$$

The translations $\mathbf{R}_n$ carry A sites into A sites and B sites into B sites, but no lattice translation interchanges inequivalent A and B sites. Hence the complete atomic arrangement is not itself a one-point Bravais lattice, although its translational skeleton is Bravais.

The upper panels of the following diagram illustrate these two cases. The lower panels show the requested planes in one cubic unit cell.



- (ii) In a cubic unit cell, the representative plane (hkl) cuts the axes at

$$x = \frac{a}{h}, \quad y = \frac{a}{k}, \quad z = \frac{a}{l},$$

with a zero index indicating that the plane is parallel to the corresponding axis.

For the three specified planes:

$$(100) : \quad \frac{x}{a} = 1 \implies x = a.$$

It is the face perpendicular to the positive x -axis and parallel to the yz -plane. Its intercepts are (a, ∞, ∞) .

$$(110) : \quad \frac{x}{a} + \frac{y}{a} = 1 \implies x + y = a.$$

It cuts the positive x - and y -axes at a and is parallel to the z -axis. Its intercepts are (a, a, ∞) .

$$(111) : \quad \frac{x}{a} + \frac{y}{a} + \frac{z}{a} = 1 \implies x + y + z = a.$$

It cuts all three positive axes at a , so the portion inside the unit cell is the triangle joining $(a, 0, 0)$, $(0, a, 0)$, and $(0, 0, a)$.

In a cubic crystal, the normal to a plane (hkl) is parallel to the crystallographic direction $[hkl]$. Thus the normals to these planes point along $[100]$, $[110]$, and $[111]$, respectively.

- (iii) The given intercepts are

$$x = a, \quad y = \frac{b}{2}, \quad z = 3c.$$

Measured in units of the corresponding axial lattice constants, the intercepts are

$$\left(1, \frac{1}{2}, 3\right).$$

Taking their reciprocals gives

$$\left(1, 2, \frac{1}{3}\right).$$

Multiplication by the least common multiple 3 clears the fraction:

$$3 \left(1, 2, \frac{1}{3}\right) = (3, 6, 1).$$

Since 3, 6, and 1 have no common integral factor, these are already the smallest relatively prime integers. Therefore the Miller indices are

$$\boxed{(361)}.$$

Equivalently, the plane equation obtained from the intercept form is

$$\frac{x}{a} + \frac{y}{b/2} + \frac{z}{3c} = 1,$$

or

$$3\frac{x}{a} + 6\frac{y}{b} + \frac{z}{c} = 3.$$

Its coefficients are proportional to $3 : 6 : 1$, confirming the same indices.

CONCLUSION:

A Bravais lattice is generated by integral combinations of primitive translations and has one translationally equivalent class of lattice points. A periodic non-Bravais arrangement requires a basis containing two or more inequivalent sites attached to each Bravais-lattice point.

In the stated positive-axis convention, the cubic planes are

$$(100) : x = a$$

$$(110) : x + y = a$$

$$(111) : x + y + z = a$$

with normals directed along $[100]$, $[110]$, and $[111]$, respectively. These relations assume a cubic cell with mutually perpendicular axes and equal lattice parameter a .

For intercepts a , $b/2$, and $3c$, the reciprocal-intercept construction gives the dimensionless, relatively prime Miller indices

$$(361).$$

CSE • 2024 • 10 MARKS

Q7. The spacing between successive (100) planes in sodium chloride is $1 \cdot 41 \text{ \AA}$. X-rays incident on the surface of the crystal are found to give rise to second order Bragg reflections at a glancing angle 10° . Calculate the wavelength of X-ray radiations.

INTRODUCTION:

The wavelength is determined using Bragg's law,

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

where d is the spacing between successive reflecting planes, n is the order of reflection, and θ is the glancing angle between the incident X-ray beam and the crystal planes. Here,

$$d = 1.41 \text{ \AA}, \quad n = 2, \quad \theta = 10^\circ,$$

with $1 \text{ \AA} = 10^{-10} \text{ m}$.

SOLUTION:

Substituting the given values in Bragg's law,

$$2\lambda = 2(1.41 \text{ \AA}) \sin 10^\circ.$$

Hence,

$$\lambda = 1.41 \text{ \AA} \times \sin 10^\circ.$$

Using

$$\sin 10^\circ = 0.17365,$$

we obtain

$$\lambda = (1.41)(0.17365) \text{ \AA} = 0.24485 \text{ \AA}.$$

Therefore, to three significant figures,

$$\lambda = 0.245 \text{ \AA}.$$

In SI units,

$$\lambda = 0.245 \times 10^{-10} \text{ m} = 2.45 \times 10^{-11} \text{ m}.$$

The result also satisfies the Bragg-reflection condition $n\lambda \leq 2d$, since

$$2\lambda = 0.490 \text{ \AA} < 2d = 2.82 \text{ \AA}.$$

CONCLUSION:

The wavelength of the incident X-ray radiation is

$$\lambda = 0.245 \text{ \AA} = 2.45 \times 10^{-11} \text{ m}.$$

IFoS • 2024 • 8 MARKS

Q8. Consider the planes with indices (1 0 0) and (0 0 1); the lattice is f.c.c., and the indices refer to the conventional cubic cell. What are the indices of these planes when referred to the primitive axes: $\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y})$, $\vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z})$ and $\vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x})$?

INTRODUCTION:

The task is to transform the Miller indices from the conventional cubic basis

$$\vec{a} = a\hat{x}, \quad \vec{b} = a\hat{y}, \quad \vec{c} = a\hat{z}$$

to the given primitive f.c.c. basis. Let a position vector be written in primitive coordinates as

$$\vec{r} = u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3.$$

The Miller indices of a plane are obtained from the reciprocals of its intercepts on the chosen crystallographic axes, with the resulting triplet reduced to the smallest integers. Equivalently, if a plane has conventional indices (hkl) , its orientation is specified by the covector

$$\vec{G} = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z}).$$

Its components with respect to the primitive reciprocal basis are determined by

$$h'_i = \frac{\vec{G} \cdot \vec{a}_i}{2\pi}.$$

SOLUTION:

For the given primitive vectors,

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y}), \quad \vec{a}_2 = \frac{a}{2}(\hat{y} + \hat{z}), \quad \vec{a}_3 = \frac{a}{2}(\hat{z} + \hat{x}),$$

the primitive reciprocal components of a conventional plane (hkl) are

$$\begin{aligned} h'_1 &= \frac{\vec{G} \cdot \vec{a}_1}{2\pi} = \frac{h+k}{2}, \\ h'_2 &= \frac{\vec{G} \cdot \vec{a}_2}{2\pi} = \frac{k+l}{2}, \\ h'_3 &= \frac{\vec{G} \cdot \vec{a}_3}{2\pi} = \frac{l+h}{2}. \end{aligned}$$

Thus,

$$(hkl)_{\text{cubic}} \longrightarrow \left(\frac{h+k}{2}, \frac{k+l}{2}, \frac{l+h}{2} \right)_{\text{primitive}}.$$

For the (100) plane,

$$(100)_{\text{cubic}} \longrightarrow \left(\frac{1}{2}, 0, \frac{1}{2} \right)_{\text{primitive}}.$$

Clearing the common denominator and reducing to the smallest integers gives

$$\left(\frac{1}{2}, 0, \frac{1}{2} \right) \sim (101).$$

The same result follows directly from the plane equation. Since

$$\vec{r} = \frac{a}{2} [(u_1 + u_3)\hat{x} + (u_1 + u_2)\hat{y} + (u_2 + u_3)\hat{z}],$$

the representative cubic plane $x = a$ becomes

$$\frac{a}{2}(u_1 + u_3) = a \implies u_1 + u_3 = 2.$$

Its primitive-axis intercepts are $(2, \infty, 2)$, whose reciprocals are

$$\left(\frac{1}{2}, 0, \frac{1}{2} \right) \sim (101).$$

For the (001) plane,

$$(001)_{\text{cubic}} \longrightarrow \left(0, \frac{1}{2}, \frac{1}{2} \right)_{\text{primitive}}.$$

Therefore,

$$\left(0, \frac{1}{2}, \frac{1}{2} \right) \sim (011).$$

Indeed, the representative plane $z = a$ gives

$$\frac{a}{2}(u_2 + u_3) = a \implies u_2 + u_3 = 2,$$

so its primitive-axis intercepts are $(\infty, 2, 2)$ and their reciprocals yield the same indices.

CONCLUSION:

When referred to the given primitive axes, the plane orientations are

$$(100)_{\text{cubic}} \equiv (101)_{\text{primitive}}$$

$$(001)_{\text{cubic}} \equiv (011)_{\text{primitive}}.$$

For the particular representative planes $x = a$ and $z = a$, the unreduced reciprocal-intercept triplets are respectively

$$\left(\frac{1}{2}, 0, \frac{1}{2} \right) \quad \text{and} \quad \left(0, \frac{1}{2}, \frac{1}{2} \right);$$

their conventional integer Miller-index forms are (101) and (011) .

CSE • 2023 • 10 MARKS

Q9. Derive diffraction conditions using reciprocal lattice concept. What are these conditions known as ?

INTRODUCTION:

Consider a crystal whose direct lattice is generated by the primitive translation vectors

$$\mathbf{a}_1, \quad \mathbf{a}_2, \quad \mathbf{a}_3,$$

so that every lattice point is at

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3, \quad n_1, n_2, n_3 \in \mathbb{Z}.$$

The reciprocal primitive vectors are defined, using the 2π convention, by

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}.$$

Thus every reciprocal-lattice vector has the form

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3, \quad h, k, l \in \mathbb{Z}.$$

Let a monochromatic plane wave of wavelength λ be incident on the crystal with wave vector

$$\mathbf{k}_i = \frac{2\pi}{\lambda} \hat{\mathbf{s}}_i,$$

and let the elastically scattered wave have wave vector

$$\mathbf{k}_f = \frac{2\pi}{\lambda} \hat{\mathbf{s}}_f.$$

The scattering vector is taken to be

$$\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i.$$

The required diffraction condition follows by demanding constructive interference between waves scattered from all translationally equivalent unit cells.

SOLUTION:

For an atom situated at $\mathbf{r}$, the incident wave contributes a phase factor

$$\exp(i\mathbf{k}_i \cdot \mathbf{r}),$$

whereas propagation of the scattered wave toward the observation direction contributes

$$\exp(-i\mathbf{k}_f \cdot \mathbf{r}).$$

Consequently, apart from the atomic scattering factor, the amplitude from that atom contains

$$\exp[-i(\mathbf{k}_f - \mathbf{k}_i) \cdot \mathbf{r}] = \exp(-i\mathbf{q} \cdot \mathbf{r}).$$

Let ρ_μ denote the position of the μ -th atom within a unit cell. The position of the corresponding atom in the cell translated by $\mathbf{R}$ is

$$\mathbf{r}_{\mu,\mathbf{R}} = \mathbf{R} + \rho_\mu.$$

The total scattered amplitude can therefore be written in the form

$$A(\mathbf{q}) = \sum_{\mathbf{R}} \sum_{\mu} f_{\mu}(\mathbf{q}) \exp[-i\mathbf{q} \cdot (\mathbf{R} + \rho_{\mu})].$$

Separating the unit-cell and lattice contributions gives

$$A(\mathbf{q}) = \sum_{\mu} f_{\mu}(\mathbf{q}) e^{-i\mathbf{q} \cdot \rho_{\mu}} \sum_{\mathbf{R}} e^{-i\mathbf{q} \cdot \mathbf{R}},$$

$\underbrace{\hspace{1.5cm}}_{F(\mathbf{q})}$

$\underbrace{\hspace{1.5cm}}_{S(\mathbf{q})}$

where $F(\mathbf{q})$ is the structure factor and $S(\mathbf{q})$ is the lattice sum.

For a crystal containing N_1, N_2, N_3 cells along the three primitive directions,

$$S(\mathbf{q}) = \prod_{j=1}^3 \left[\sum_{n_j=0}^{N_j-1} e^{-in_j \mathbf{q} \cdot \mathbf{a}_j} \right].$$

Each factor is a geometric series:

$$\sum_{n=0}^{N-1} e^{-inx} = e^{-i(N-1)x/2} \frac{\sin(Nx/2)}{\sin(x/2)}.$$

Its magnitude becomes of order N , rather than remaining bounded, when

$$x = 2\pi m, \quad m \in \mathbb{Z}.$$

Hence sharp diffraction maxima occur when

$$\mathbf{q} \cdot \mathbf{a}_1 = 2\pi h, \quad \mathbf{q} \cdot \mathbf{a}_2 = 2\pi k, \quad \mathbf{q} \cdot \mathbf{a}_3 = 2\pi l,$$

where h, k, l are integers.

Expanding $\mathbf{q}$ in the reciprocal basis,

$$\mathbf{q} = x_1 \mathbf{b}_1 + x_2 \mathbf{b}_2 + x_3 \mathbf{b}_3,$$

and taking scalar products with the direct primitive vectors gives

$$\mathbf{a}_1 \cdot \mathbf{q} = 2\pi x_1, \quad \mathbf{a}_2 \cdot \mathbf{q} = 2\pi x_2, \quad \mathbf{a}_3 \cdot \mathbf{q} = 2\pi x_3.$$

Comparison with the constructive-interference conditions yields

$$x_1 = h, \quad x_2 = k, \quad x_3 = l.$$

Therefore,

$$\mathbf{k}_f - \mathbf{k}_i = \mathbf{q} = \mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3.$$

Thus diffraction occurs only when the momentum-transfer wave vector is a reciprocal-lattice vector.

Equivalently, writing

$$\mathbf{k}_i = \frac{2\pi}{\lambda} \hat{\mathbf{s}}_i, \quad \mathbf{k}_f = \frac{2\pi}{\lambda} \hat{\mathbf{s}}_f,$$

the three scalar conditions become

$$\mathbf{a}_1 \cdot (\hat{\mathbf{s}}_f - \hat{\mathbf{s}}_i) = h\lambda,$$

$$\mathbf{a}_2 \cdot (\hat{\mathbf{s}}_f - \hat{\mathbf{s}}_i) = k\lambda,$$

$$\mathbf{a}_3 \cdot (\hat{\mathbf{s}}_f - \hat{\mathbf{s}}_i) = l\lambda.$$

These are the three scalar forms of the diffraction condition.

For elastic diffraction,

$$|\mathbf{k}_f| = |\mathbf{k}_i| = \frac{2\pi}{\lambda}.$$

Since $\mathbf{k}_f = \mathbf{k}_i + \mathbf{G}$, this requires

$$|\mathbf{k}_i + \mathbf{G}|^2 = |\mathbf{k}_i|^2,$$

and hence

$$2\mathbf{k}_i \cdot \mathbf{G} + G^2 = 0.$$

Geometrically, the endpoint of $\mathbf{k}_f$ must lie both on a sphere of radius $2\pi/\lambda$, centred at the tail of $\mathbf{k}_i$, and at a reciprocal-lattice point. This is the reciprocal-space construction of the diffraction condition, commonly called the Ewald-sphere construction.

The equivalence with Bragg's law follows by associating $\mathbf{G}$ with a family of lattice planes normal to $\mathbf{G}$. If their spacing is d , then

$$|\mathbf{G}| = \frac{2\pi}{d}.$$

Let θ be the glancing angle between the incident beam and these planes. For the reflecting orientation,

$$\mathbf{k}_i \cdot \mathbf{G} = -|\mathbf{k}_i||\mathbf{G}| \sin \theta.$$

Substitution in

$$2\mathbf{k}_i \cdot \mathbf{G} + G^2 = 0$$

gives

$$2|\mathbf{k}_i||\mathbf{G}| \sin \theta = G^2.$$

Using

$$|\mathbf{k}_i| = \frac{2\pi}{\lambda}, \quad |\mathbf{G}| = \frac{2\pi}{d},$$

one obtains

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

If the momentum transfer is the n -th multiple of the reciprocal vector corresponding to planes of spacing d , the result is

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

which is Bragg's law.

The lattice condition determines the allowed positions of diffraction maxima, while the structure factor $F(\mathbf{G})$ determines their relative intensities and may make some otherwise allowed reflections vanish.

CONCLUSION:

The reciprocal-lattice diffraction condition is

$$\mathbf{k}_f - \mathbf{k}_i = \mathbf{G}, \quad \mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3, \quad h, k, l \in \mathbb{Z},$$

or, equivalently,

$$\mathbf{a}_1 \cdot (\mathbf{k}_f - \mathbf{k}_i) = 2\pi h, \quad \mathbf{a}_2 \cdot (\mathbf{k}_f - \mathbf{k}_i) = 2\pi k, \quad \mathbf{a}_3 \cdot (\mathbf{k}_f - \mathbf{k}_i) = 2\pi l.$$

These are known as the *Laue diffraction conditions* or *Laue equations*. For elastic scattering they are equivalent to Bragg's law,

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

Physically, a diffraction maximum is possible when the scattering vector terminates at a reciprocal-lattice point; its observable intensity is then governed by the unit-cell structure factor.

IFoS • 2023 • 10 MARKS

Q10. Draw the crystal structure of CaF_2 indicating the positions of cations and anions. What are their respective coordination numbers?

INTRODUCTION:

CaF_2 crystallizes in the cubic fluorite structure. We describe one conventional cubic unit cell of edge length a , with Cartesian axes along its edges and the origin at a corner. Fractional coordinates (x, y, z) denote the position

$$\mathbf{r} = a(x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}).$$

The Ca^{2+} ions form a face-centred cubic lattice, while the F^- ions occupy all the tetrahedral interstitial sites of that lattice. The required coordination numbers follow by identifying the nearest neighbours of each ion.

SOLUTION:

The Ca^{2+} ions occupy the corners and face centres of the conventional cubic cell. Representative fractional coordinates are

$$(0, 0, 0), \quad \left(0, \frac{1}{2}, \frac{1}{2}\right), \quad \left(\frac{1}{2}, 0, \frac{1}{2}\right), \quad \left(\frac{1}{2}, \frac{1}{2}, 0\right),$$

together with lattice-equivalent positions on the cell boundary.

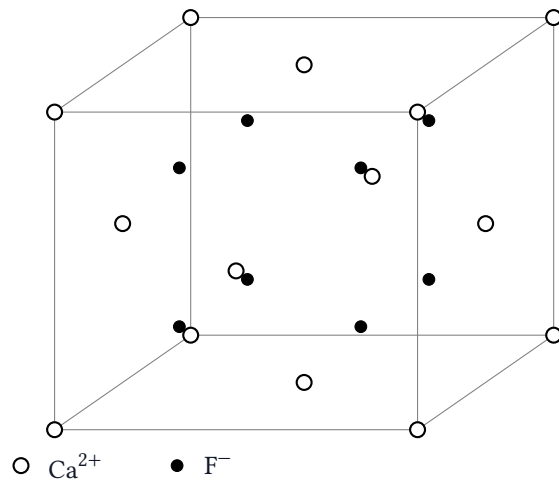
All eight tetrahedral sites are occupied by F^- ions:

$$(x, y, z), \quad x, y, z \in \left\{\frac{1}{4}, \frac{3}{4}\right\}.$$

Thus the fluorine-ion positions include

$$\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right), \left(\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right), \left(\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right), \left(\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right),$$

and the four positions obtained by the remaining choices of $\frac{1}{4}$ and $\frac{3}{4}$.



The number of calcium ions belonging to one conventional cell is

$$8\left(\frac{1}{8}\right) + 6\left(\frac{1}{2}\right) = 4,$$

whereas all eight fluoride ions shown lie inside the cell:

$$N_{\text{F}} = 8.$$

Hence

$$N_{\text{Ca}} : N_{\text{F}} = 4 : 8 = 1 : 2,$$

as required by the formula CaF_2 .

For a calcium ion at the origin, the nearest fluoride ions are at relative positions

$$\frac{a}{4}(\pm 1, \pm 1, \pm 1).$$

There are $2^3 = 8$ such choices, all at the same distance

$$d_{\text{Ca-F}} = \sqrt{\left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2} = \frac{\sqrt{3}a}{4}.$$

Therefore each Ca^{2+} ion is surrounded by eight F^- ions situated at the vertices of a cube.

Consider next the fluoride ion at

$$\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right).$$

Its four nearest calcium ions are at

$$(0, 0, 0), \quad \left(0, \frac{1}{2}, \frac{1}{2}\right), \quad \left(\frac{1}{2}, 0, \frac{1}{2}\right), \quad \left(\frac{1}{2}, \frac{1}{2}, 0\right).$$

Each is at distance $\sqrt{3}a/4$ from the fluoride ion, and these four calcium ions form the vertices of a tetrahedron. Thus each F^- ion has four nearest Ca^{2+} neighbours.

The coordination counts are also mutually consistent: with four calcium and eight fluoride ions per cell,

$$4(8) = 8(4) = 32,$$

so both descriptions count the same number of nearest-neighbour Ca – F contacts.

CONCLUSION:

In the fluorite structure of CaF_2 , the Ca^{2+} ions form a face-centred cubic lattice and the F^- ions occupy all eight tetrahedral sites of each conventional unit cell. Each Ca^{2+} ion is cubically coordinated by eight F^- ions, whereas each F^- ion is tetrahedrally coordinated by four Ca^{2+} ions. Therefore,

$CN(Ca^{2+}) = 8, \quad CN(F^-) = 4.$



UPSC PHYSICS OPTIONAL for CSE & IFoS

ABHI PHYSICS

A SYSTEMATIC ARCHIVE OF SOLVED PHYSICS OPTIONAL PYQs

Detailed, source-tagged solutions arranged for focused study,
conceptual reconstruction and reliable examination reference.

SSP and Electronic Devices

41 YEARS | 1986–2026

10 SOLVED QUESTIONS | CSE + IFoS

Published by Abhi Physics

For Civil Services and Indian Forest Service Examinations

www.abhi-physics.com