ESO 205A (P)

Nature and Properties of Materials

Interaction session: 6:30 – 7:20 pm Thursdays

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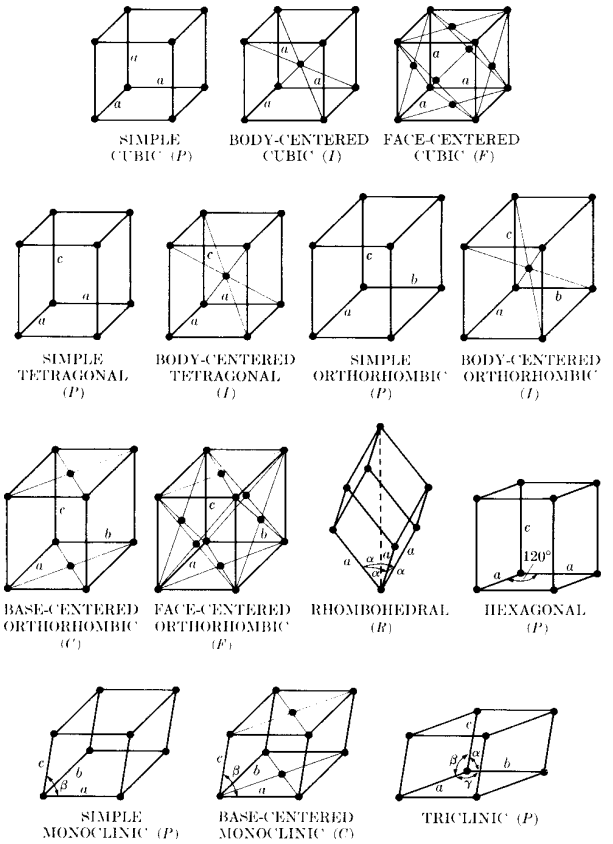
Module 1

Crystal structure
and
X-ray diffraction

14 Bravais lattice in 3D

- 7 crystal classes
  - Cubic (P, I, F)
  - Tetragonal (P, I)
  - Orthorhombic (P, I, B, F)
  - Rhombohedral (P)
  - Hexagonal (P)
  - Monoclinic (P, B)
  - Triclinic (P)

- 4 type of unit cells
  - Primitive (P)
  - Body centered (I)
  - Base centered (A, B, C)
  - Face centered (F)



Crystal systems

Minimum Symmetry

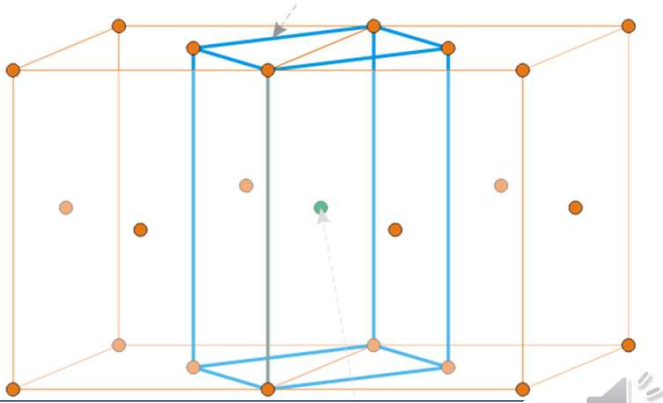
Crystal System:	Minimum Symmetry:
Triclinic	No Symmetry
Monoclinic	1 A2
Trigonal	1 A3
Tetragonal	1 A4
Hexagonal	1 A6
Orthorhombic	3 A2
Cubic	4 A3

Crystal System	Axial and Angular Relationships	Bravais Lattice*	No. of lattice points/cell
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^o$	Simple Cubic (P)	1
		Body Centred Cubic (I)	2
		Face Centred Cubic (F)	4
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^o$	Simple Tetragonal (P)	1
		Body Centred Tetragonal (I)	2
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^o$	Simple Orthorhombic (P)	1
		Body Centred Orthorhombic (I)	2
		Base Centred Orthorhombic (C)	2
		Face Centred Orthorhombic (F)	4
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^o, \gamma = 12O^o$	Simple Hexagonal (P)	1
Rhombohedral	$a = b = c$ $\alpha = \beta = \gamma \neq 90^o$	Simple Rhombohedral (P)	1
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^o \neq \beta$	Simple Monoclinic (P)	1
		Base Centred Monoclinic (C)	2
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^o$	Simple Triclinic (P)	1

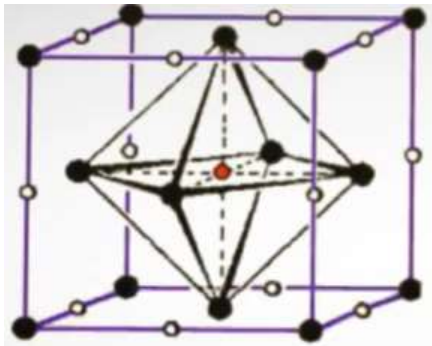
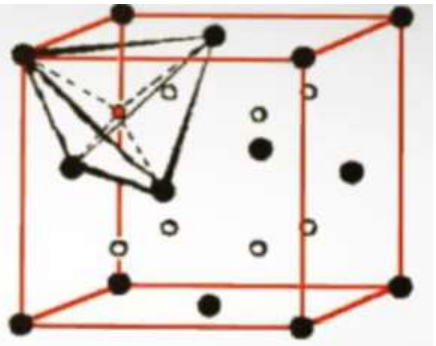
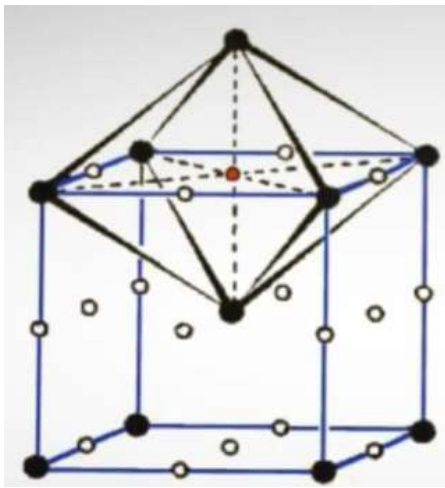
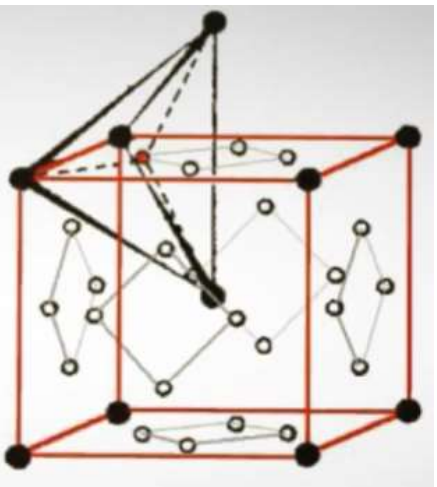
- Number of lattice points per unit cell in 3D
  - Primitive (P): 1
  - Body centered (I): 2
  - Base centered (A, B, C): 2
  - Face centered (F): 4

Prove to your self that only 14 Bravais lattices are possible

Face centered tetragonal = Body Centered Tetragonal

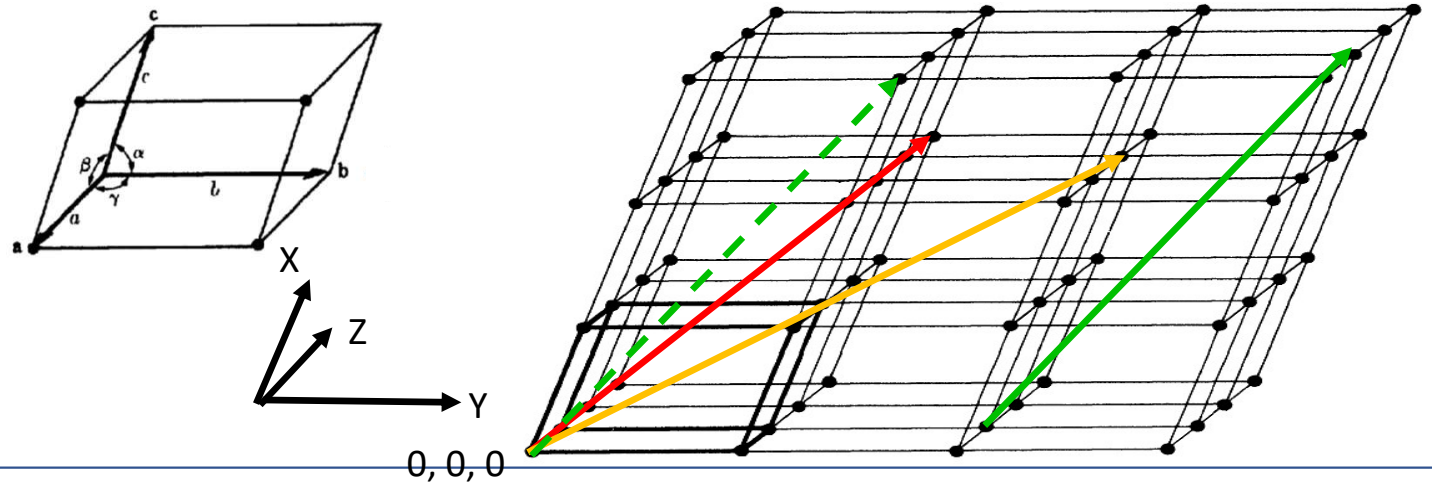


Voids

	Octahedral	Tetrahedral
FCC		
BCC		

Crystallographic directions

- Red arrow [213]
- Orange arrow [222] not 2 * [111]
- Green arrow foes not pass through origin so draw a parallel line (dashed) from origin and get [310]



Crystallographic planes

- Crystalline materials in 3D have different crystallographic planes
- Different planes have different properties in the same crystal
- Planes are essentially surfaces
- Number of atoms per plane different
- Understanding of planes and the sub dimensional information like number of atoms, and planar packing density important
- Same is true for directions

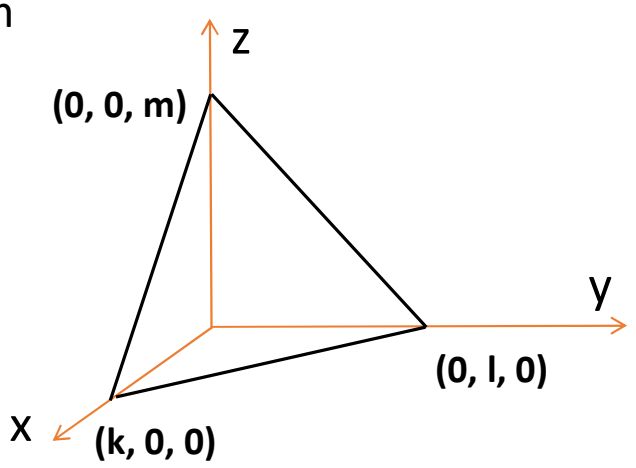
Miller indices for planes

1. Intercept with X, Y, and Z axis
2. (k, 0, 0); (0, l, 0) and (0, 0, m)
3. Determine k/a, l/b, m/c, where a, b, c are lattice parameters along X, Y and Z resp.
4. Determine a/k, b/l, c/m
5. If fractions then multiply each of these by lowest common multiple (LCM), let say it is N

Or, if the three numbers have a common factor then divide them with this highest common factor (HCF)

The Miller indices of the plane are

$$\left(\frac{a}{k}N\ \frac{b}{l}N\ \frac{c}{m}N\right)$$



➢ Bragg equation

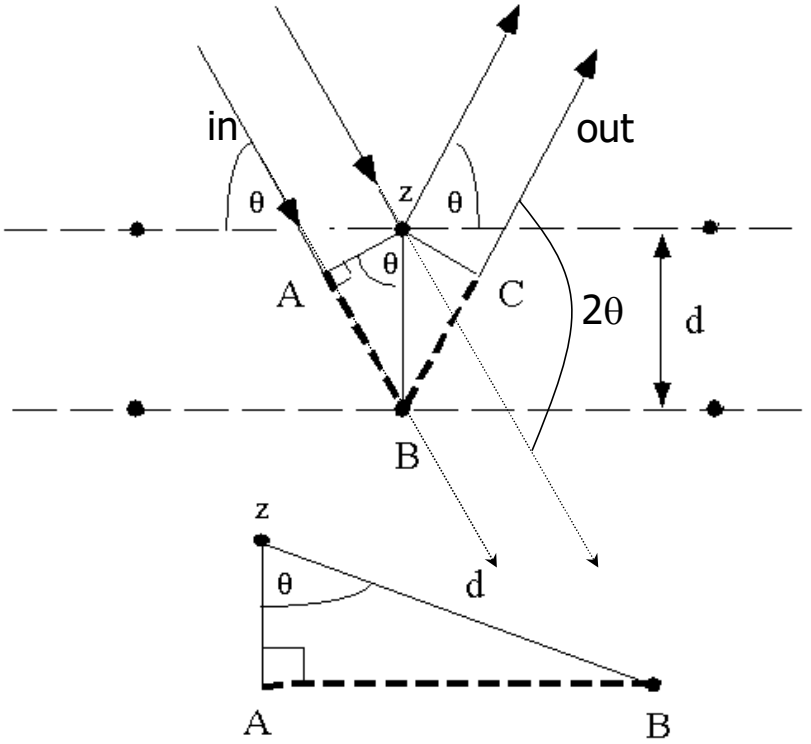
$n\lambda = 2d.\sin\theta$

n: Order of reflection

d: Plane spacing

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

θ: Bragg Angle



$\theta_{in} = \theta_{out}$

Path difference must be integral multiples of the wavelength for constructive interference

Scattering of X-rays by an unit cell

Real space

Reciprocal space

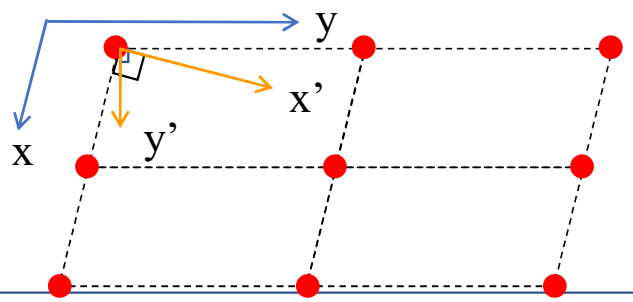
Crystal Lattice

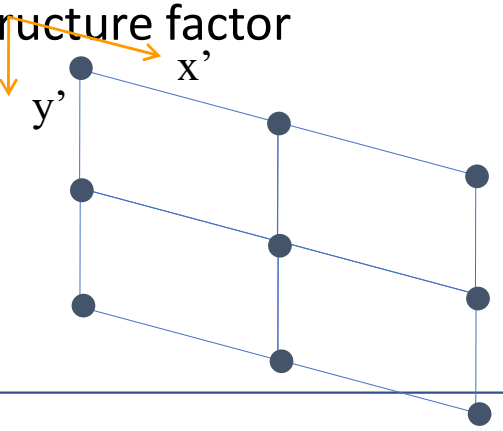
Reciprocal Lattice

Crystal structure → Diffraction pattern

Unit cell content

Structure factor





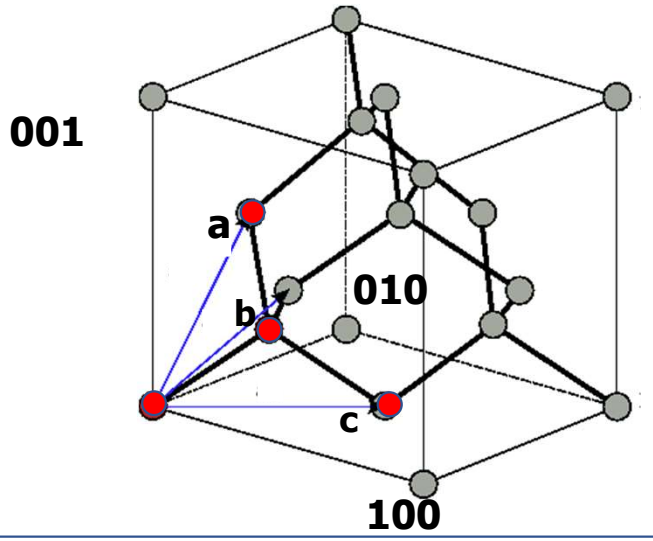
Reciprocal space

$$a^* = \frac{b \times c}{a \bullet (b \times c)}$$

$$b^* = \frac{c \times a}{a \bullet (b \times c)}$$

$$c^* = \frac{a \times b}{a \bullet (b \times c)}$$

Reciprocal lattice of FCC is BCC and vice versa



Structure factor

- Link crystal structure with diffraction pattern
- Position and intensity of peaks $$F_{hkl} = \sum_{1}^{N} f_n e^{2\pi i(hu_n + kv_n + lw_n)}$$
- Atomic positions decide presence of hkl peak
- SC: (0, 0, 0), so all peaks possible
- BCC: (0, 0, 0) and (0.5, 0.5, 0.5) so only h+k+l = even peaks possible
- Remember $e^{2n\pi i} = 1$, where n is an integer
- $e^{p\pi i} = -1$, if p is odd

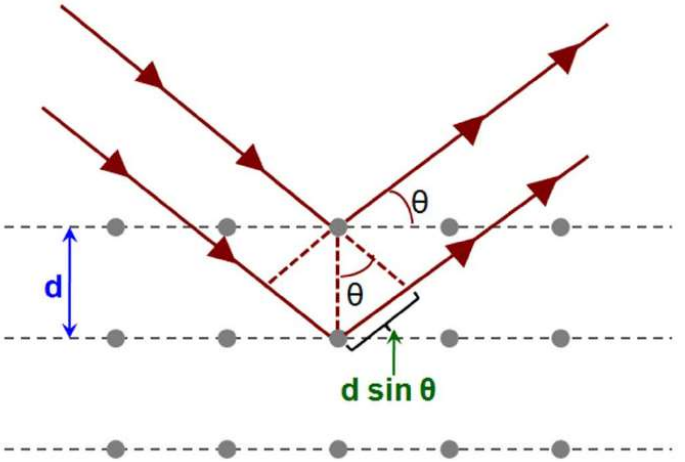
Bravais Lattice	Reflections possibly present	Reflections necessarily absent
Simple	All	None
Body Centered	(h+k+l): Even	(h+k+l): Odd
Face Centered	h, k, and l unmixed i.e. all odd or all even	h, k, and l: mixed

Permitted Reflections

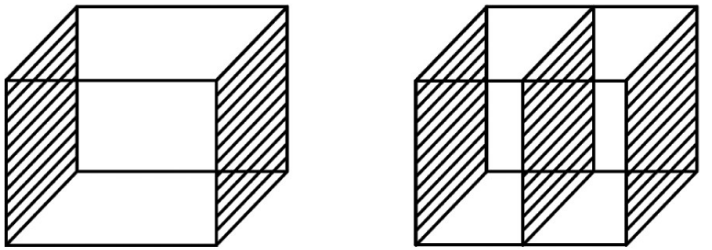
Simple Cubic	(100), (110), (111), (200), (210), (211), (220), (300), (221) ……
BCC	(110), (200), (211), (220), (310), (222)….
FCC	(111), (200), (220), (311)…..

Physical interpretation

- 100 peak in SC not in BCC and FCC
- Bragg equation derivation
- 100 plan^{2}e in SC has 1 atom (4 * 0.25) for a^2 area and 200 plane has zero atom for area of a. $d_{100} = 2d_{200} = a$



- Constructive interference between 100 planes so 100 peak in SC
- In BCC 1 atom for a^2 area for 100 plane and 1 atom per a^2 area for 200 plane. Destructive interference so no 100 peak but 200 peak
- Similar analogy for FCC



- From hkl to theta
- We can measure 1/10th of a nanometer
- In fact we can get a precision of 1/1000th of a nanometer
- s = 1, 2, 3…6, 8 for SC (no 7)
- s = 2, 4, 6, 8 for BCC
- s = 3, 4, 8, 11, 12, 16….

$$\lambda = 2dSin\theta$$

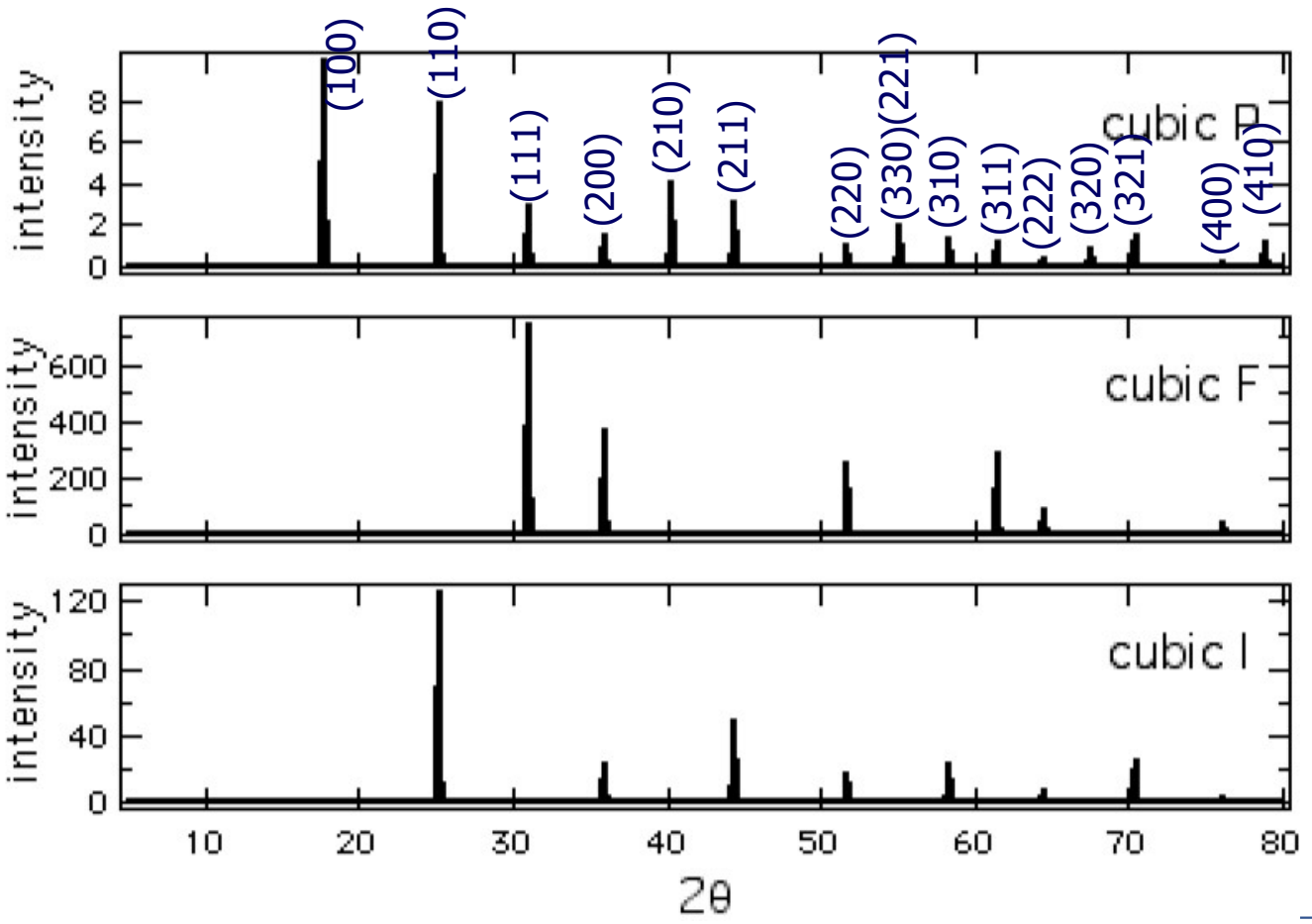
$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

$$\lambda^2 = \frac{4a^2 \sin^2 \theta}{h^2 + k^2 + l^2}$$

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

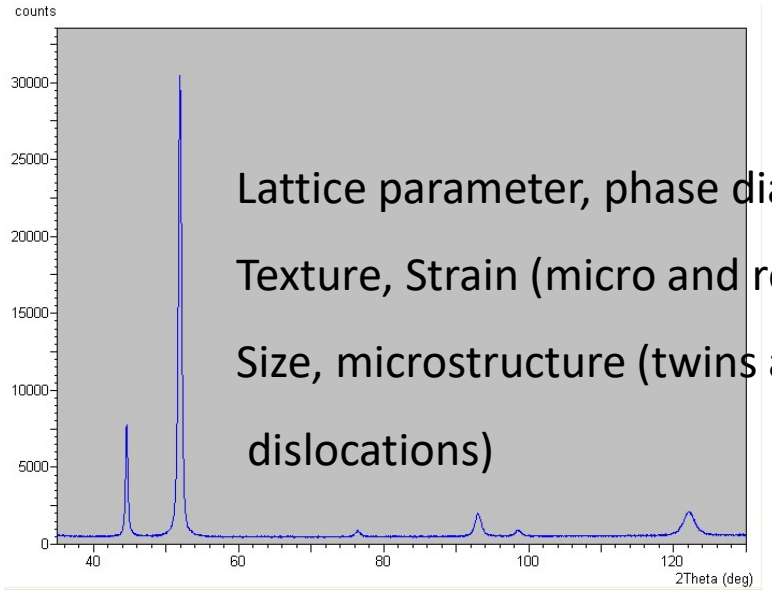
$$s = (h^2 + k^2 + l^2) \propto \sin^2 \theta$$

XRD pattern for Cubic Crystals



Intensity of X-ray pattern

- structure factor (F^2)
- polarization factor
- multiplicity factor
- Lorentz factor
- absorption factor
- temperature factor



Lattice parameter, phase diagrams

Texture, Strain (micro and residual)

Size, microstructure (twins and dislocations)

Module 1 Assignment

- Visit the webpage and take snapshots of SC, BCC and FCC crystals from different views. Mention the plane or direction along which you are acquiring the snapshot.

https://jeremyberchtold.com/UnitCellVisualizer/

- Visualize 4 distinct planes such that h ≠ k ≠ l using this tool

http://calistry.org/calculate/latticePlanesMillerIndices

- Index the X-ray diffraction pattern provided in the file. Find the crystal structure and lattice parameter

Stay safe and take care
Get vaccinated

Thank you