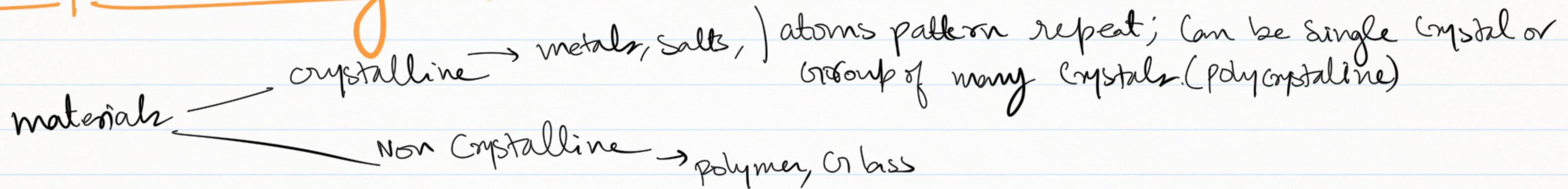


Crystal Geometry



Crystal \rightarrow 3D arrangement of atoms

Lattice \rightarrow imaginary mathematically observed points in a Space

motif \rightarrow a group of atoms placed at lattice points.

$$\text{Crystal} = \text{lattice} + \text{motif}$$

Lattice translation \rightarrow a vector from one lattice point to another lattice point.

Unit Cell \rightarrow Smallest set of arranged atoms which can be further multiplied to create entire crystal.

| Primitive unit cell \rightarrow where lattice point only at corners

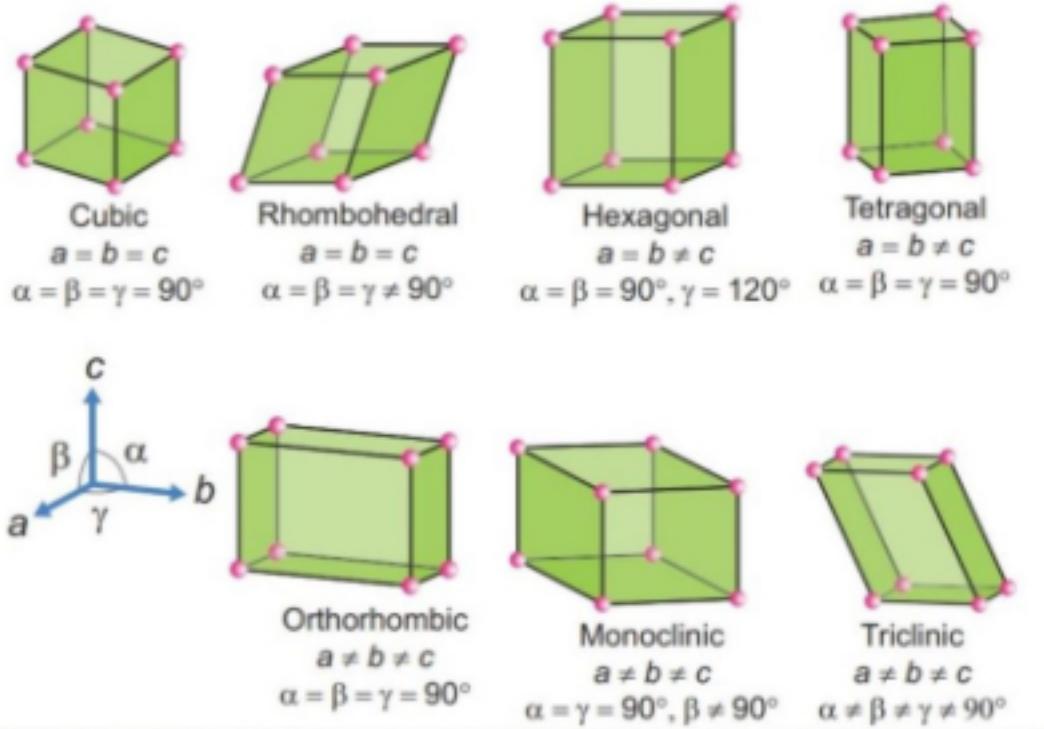
| Non-primitive unit cell \rightarrow "where don't"

7 Crystal structures \rightarrow Cubic, Rhombohedral, Hexagonal, Tetragonal, Orthorhombic, Monoclinic, Triclinic

14 bravais lattice \rightarrow $\frac{1}{3}$ + $\frac{1}{2}$ + $\frac{1}{4}$ = $\frac{1}{1}$ + $\frac{1}{4}$ + $\frac{1}{2}$ + $\frac{1}{1}$

Miller indices \rightarrow direction of planes

7 Lattice systems (Primitive)



14-Bravais-lattice

cubic			
tetragonal			
hexagonal			
orthorhombic			basis face centered
monoclinic			
trigonal			
triclinic			

Q Why No edge centred lattice →
 Ans → In a edge centred lattice, 2 edge centred lattice point won't be equivalent.

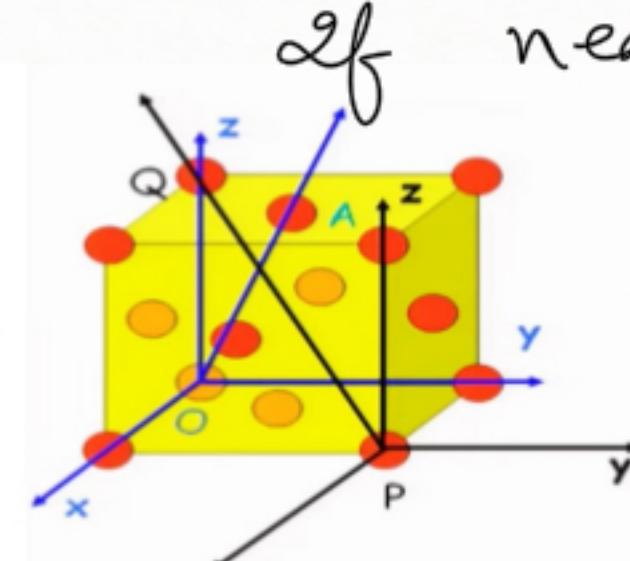


Q Why only 14 Bravais lattice, why not 28?

Ans → If we take an end centric lattice it will no longer be a unit cell as it could be further divided into similar parts to unit cells as among these 14 Bravais lattice.

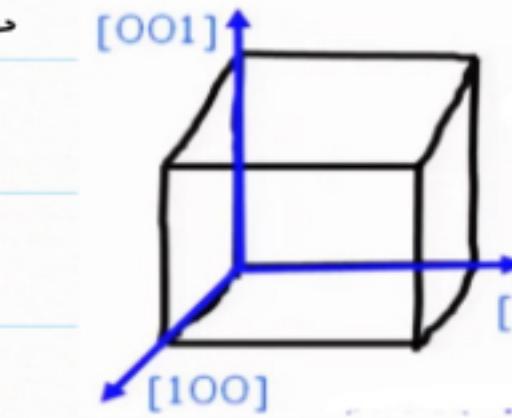
Miller Indices →

- C D | - write the vector by taking initial lattice as origin in the form $ax+by+cz$
- R I | - $[a,b,c]$ are Miller Indices of this vector.
- Y L | - Used to tell directions only, hence all parallel vectors have same Miller indices
- S E |
- T C |
- A T |
- L O |
- N S |
- write in whole numbers only; not fractions $\rightarrow \frac{1}{2}x + \frac{1}{2}y + \frac{1}{2}z \Rightarrow [1,1,2]$
- if negative, get a bar instead $\rightarrow (-)x + (-)y + (-)z \Rightarrow [\bar{1},\bar{1},\bar{1}]$



← must use coordinate system like this, facing its board in front, right hand of yours.

Miller Indices for family of directions :-

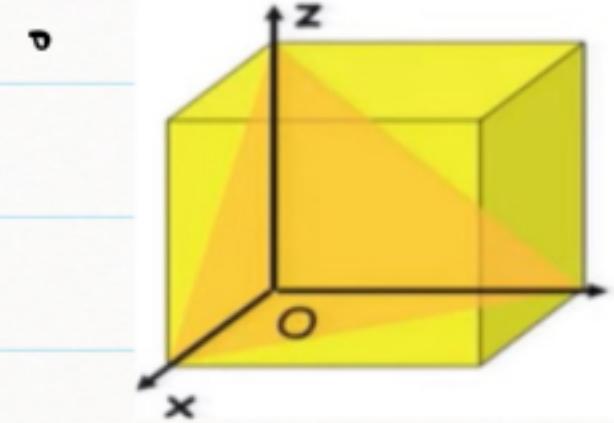


$$\langle 100 \rangle = [100], [0, 1, 0], [0, 0, 1], [-1, 0, 0], [0, -1, 0], [0, 0, -1]$$

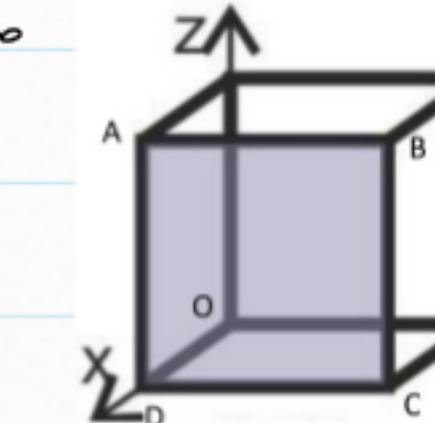
this represent all these directions (family of directions)

Miller Indices for direction of Planes:-

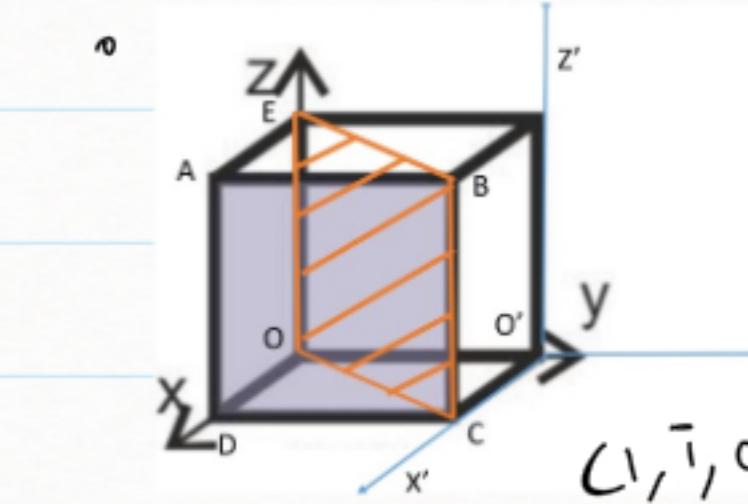
- Origin Must not be on the plane whose miller indice we are taking. A Cr-System as earlier must be taken for the Origin.
- take the intersecting points b/w given plane and coordinate axis; Reciprocal it ; change it to Smallest integer in Same Ratio ; Enclose in parenthesis



$$(1,1,1)$$



Plane: ABCD
Origin: O
Intercepts : 1 ∞∞∞
Reciprocals : 1 0 0
Smallest integers: 100
Enclose in parenthesis: (100)



$$(1,-1,0)$$

Plane: OCBE

Origin: O'
Intercepts: -1, -1, ∞
Reciprocal: 1, -1, 0
smallest int: 1, -1, 0
Parenthesis: - (1, -1, 0)

Miller Indices for family of directions of Plane



front and back face - (100), (-100)

left and right face - (010), (0-10)

top and bottom -- - (001), (00-1)

$$\{100\} = (100), (010), (001), (-100), (0-10), (00-1)$$

Interplaner Spacing \rightarrow distance b/w plane of Miller Indice h, k, l and parallel plane Consisting origin is

$$d_{h,k,l}^{\text{Cubic lattice}} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Interplaner Spacing for a family of plane (h, k, l) is Same.

Structural determination by X-Ray :-

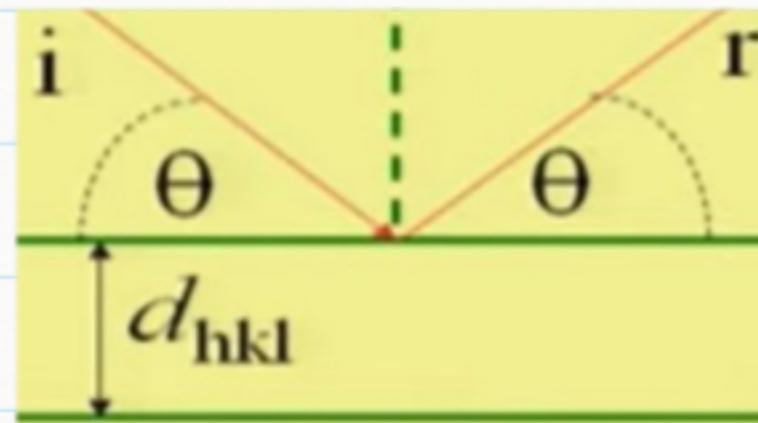
- done by diffraction
- Interatomic dis $2-3 \text{ \AA}$, hence X-ray is beam capable for diffraction



$$a \approx \lambda \text{ (wavelengtn of beam)}$$

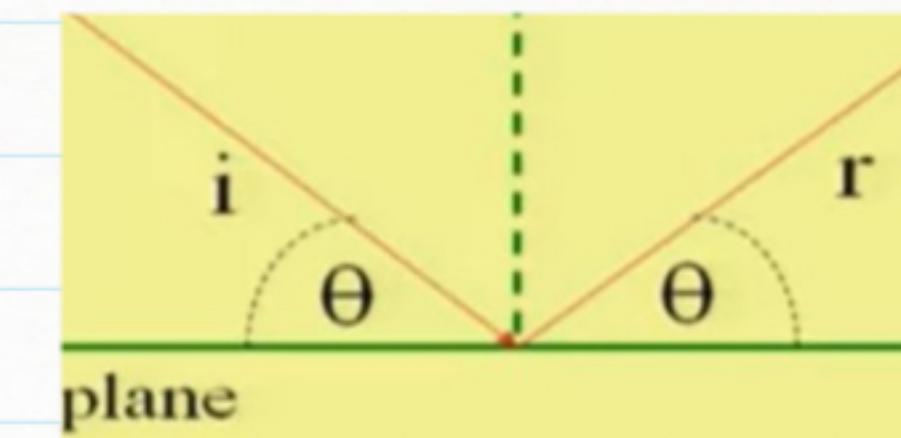
Bragg's law : for every diffracted beams, there are Sets of beams which gets reflected by some sets of Crystal lattice planes

angle of reflection = angle of incident (measured from plane); incident, reflection normal lie in same plane



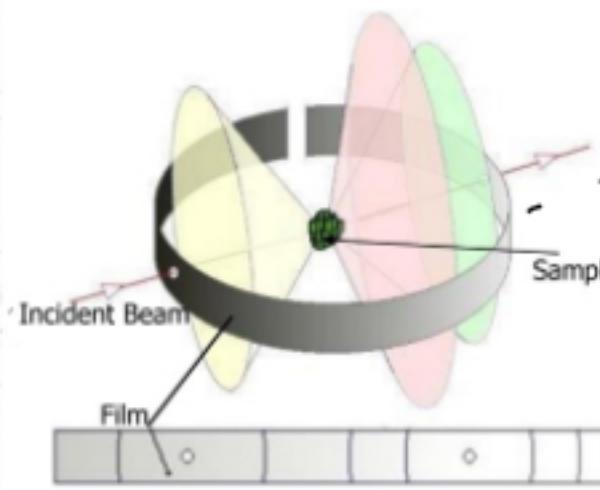
$$n\lambda = 2d_{hkl} \sin \theta \quad (\text{Bragg's law P2})$$

(* Tip $n=1$ if nothing given or strikes)



- for structural determination
 - a monochromatic beam + Many crystals in different orientation ; man decrease down to achieve bragg's.
 - a white (many wavelength) beam + single crystal at Specific Orientation
 - a monochromatic beam + Single crystal rotated at many angles.

Powder method :-



Intersections of cones giving arcs

$$S = 4R\theta \rightarrow \text{bragg's angle}$$

distance b/w two arcs

\uparrow Radius of ring

Extinction Rule for Cubic Structures

• derive the ratios of $h^2 + k^2 + l^2$ values for allowed reflections in provided crystal;
if the values ($h^2 + k^2 + l^2$) lies in these ratios:-

SC 1 : 2 : 3 : 4 : 5 : 6 : 8

BCC 1 : 2 : 3 : 4 : 5 : 6 : 7

FCC 3 : 4 : 8 : 11 : 12

DC 3 : 8 : 11 : 16

$$\frac{\sin^2 \theta}{h^2 + k^2 + l^2} = \frac{\lambda^2}{4a^2} \rightarrow \text{might be usefull at time of solving cubic crystal related prob.}$$

$(n\lambda = 2ds\sin\theta; d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}})$