

Syllabus:

- Crystal lattices
- Miller indices
- Miller-Bravais indices
- Structures of metallic, ionic and polymer crystals
- Reciprocal lattice
- X-ray diffraction techniques
- Geometric structure factor
- Numerical problems related to these topics

Introduction Slide:

- Bonds:
 - Primary: *Ionic, Metallic, Covalent*
 - Secondary: *Fluctuating Induced Dipole Bond, Polar Molecule-Induced Dipole Bonds*
- Lattice + Basis = Crystalline Structure
- **Crystallographic Structures:**
 - Cubic
 - Tetragonal
 - Orthorhombic
 - Monoclinic
 - Triclinic
 - Rhombohedral
 - Hexagonal
- Space Lattice
- 2D Lattices:
 - Square Lattice
 - Rectangular Lattice (*Rect. unit cell, centered unit cell*)
 - Hexagonal Lattice
 - Parallelogram Lattice
- **Crystallographic Restriction Theorem**
- **Unit Cells:**
 - Primitive
 - Face Centered
 - Body Centered
 - Side Centered

- Combination of unit cells and crystallographic structures: Bravais Lattices

Book: Chapters 1-3:

- Unit Cell
- Coordination Number (CN)
- Atomic Packing Factor (APF)
- **Face Centered Cubic (FCC)**
 - Eq. atoms : 4
 - $a : 2\sqrt{2} R$
 - CN : 12
 - APF : 0.74
- **Body Centered Cubic (BCC)**
 - Eq. atoms : 2
 - $a : 4R/\sqrt{3}$
 - CN: 8
 - APF: 0.68
- **Hexagonal Close Packed (HCP)**
 - Eq. atoms : 6
 - $c/a : 1.633$
 - CN : 12
 - APF : 0.74
- Cation/Anion ratios : (r_c/r_a)
 - CN 2 : < 0.155
 - CN 3 : $0.155 - 0.225$
 - CN 4: $0.225 - 0.414$
 - CN 6 : $0.414 - 0.732$
 - CN 8 : $0.732 - 1$
 - CN 12 : > 1
- NaCl
 - FCC - CN : 6
- CsCl
 - BCC - CN : 8
- ZnS
 - Tetrahedral - CN : 4
- **Density computation formula**
- Diamond
- Graphite

- Polymorphism
- Allotropy
- **Crystallographic Directions**
 - What, why
 - Notation
 - Drawing
 - Family of Directions
- **Miller-Bravais Coordination System**
 - What, why
 - Notation
 - Drawing
- Conversion from 3 to 4 indices, vice versa
 - $[u'v'w'] = [uvw]$
 - $U = n(2u' - v')/3$
 - $V = n(2v' - u')/3$
 - $W = nw'$
 - $T = -(u+v)$
- **Crystallographic Planes**
- **Miller Indices [hkl]**
- **Miller Bravais Indices [hkil]**
 - Conversion
 - $i = -(h + k)$
- Polycrystalline Materials
- Anisotropy
- Isotropy

Reciprocal Lattice PDF:

- Definition, basics
- Mathematical Definition $\rightarrow e^{i\mathbf{K} \cdot \mathbf{R}} = 1$, for \mathbf{R} of Bravais Lattice and periodicity \mathbf{K}
- Reciprocal vectors from original vectors
- Proof that reciprocal of reciprocal lattice is original lattice
- **Reciprocal Lattice of FCC**
 - BCC
 - $\mathbf{b}_1 = 4\pi/a (y + z - x) \dots$ and so on.
- **Vice versa for Reciprocal of BCC**
- Reciprocal of Reciprocal Lattice
- Volume of RL : $(2\pi)^3/v$

- Lattice Plane definition
- Family of Lattice Planes definition
- **Reciprocal Lattice Plane Theorem -- + -- Proof**
- Reciprocal Vectors as Miller Indices of Lattice Plane
- **Intercepts with crystal axes of a Lattice Plane are reciprocals of miller indices -- Proof**

X-Ray Diffraction:

- Bragg's Equation
 - $n\lambda = 2d\sin\theta$
 - Order of reflection = n
 - Assumptions
- Von Laue Approach
 - How is it different from Bragg's
 - Condition for constructive interference
 - $K = |k - k'|$
- Equivalence of Bragg's and Von Laue Condition
- **Ewald's Construction**
 - Laue's method
 - Rotating Crystal Method
 - Powder or Debye Scherrer Method
- Geometric Structure Factor
 - Mathematical Definition
 - BCC Even | Odd Proof
- https://www.researchgate.net/post/How_can_I_find_the_structure_FCC_or_BCC_etc_when_it_is_not_available_in_JCPDS
- http://physics.usask.ca/~bzulkosk/modphyslab/phys381manual/xray_diffraction_2004.pdf