

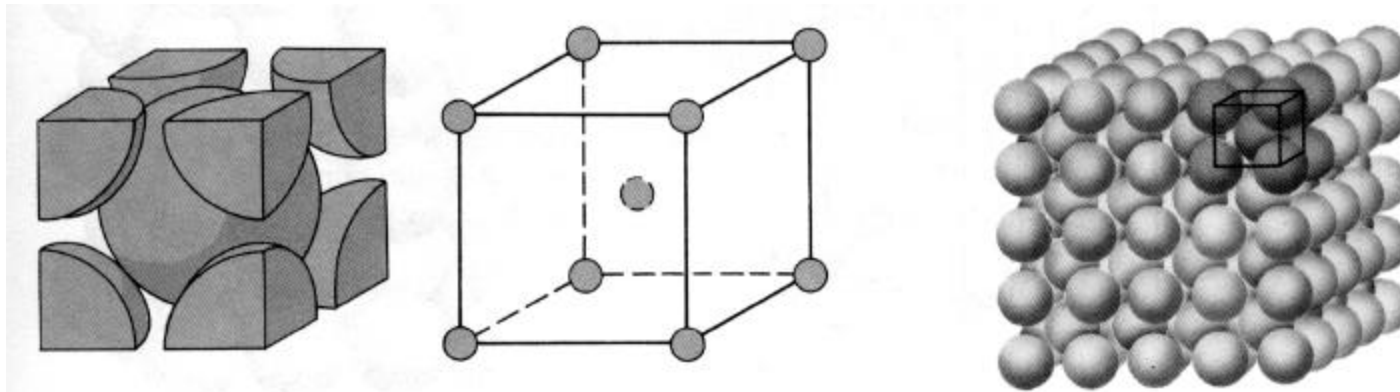
Crystalline Structures

- The atomic arrangement or crystalline structure of a material is important in determining the behavior and properties of a solid material.
- We use the Atomic Hard Sphere Model when describing the crystalline structures.

Order: Short vs. Long Range

- **No Order** - atoms or molecules are in random order
- **Short Range Order** - atoms or molecules are only arranged with their closest neighbors
- **Long Range Order** - atoms or molecules are arranged in a regular repetitive pattern or lattice.

Unit Cells



- 14 Types of unit cells also know as Bravais lattices.
- These are grouped into 7 different crystalline structures.

Lattices

- **Lattice Point** - The points that make up the unit cell.
- **Lattice Parameters** - are the dimensions of the lattice along with the angle between the sides.
- **Packing Factor** - is the volume occupied by the atoms in a unit cell.

$$P.F. = \frac{(\# \text{ of atoms/cell})(\text{volume of each atom})}{\text{volume of unit cell}}$$

Crystalline Transformation

- **Polymorphic** - a material that can have more than one crystalline structure.
- **Allotropic** - same as polymorphic but reserved for use when referring to a pure element.

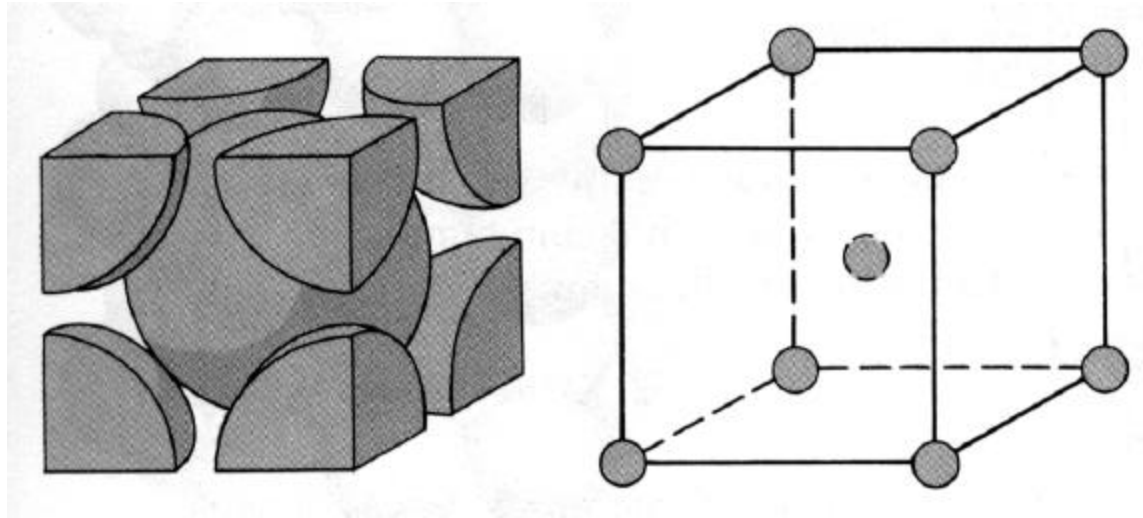
These transformations usually are associated with changes in temperatures. Iron has a BCC structure at low temp but FCC at higher temperatures.

Behavior and Crystallographic Direction

- **Anisotropic** - Physical properties depend on the crystallographic direction.
- **Isotropic** - Physical properties are independent of the crystallographic direction

Polycrystalline materials are made up of many small crystals or grains which are randomly oriented.

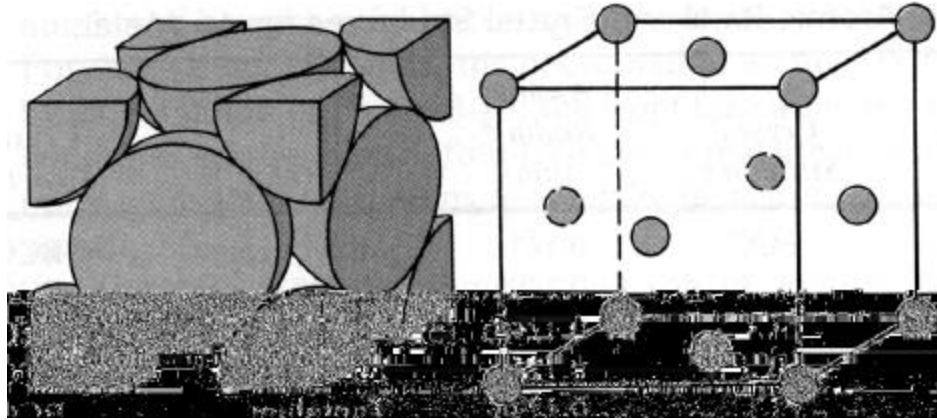
Body Centered Cubic (BCC)



- Two atoms per unit cell, one in the center and $\frac{1}{8}$ of each of the 8 corner atoms.
- Close-packed direction $\langle 111 \rangle$, diagonal from opposite corners going through the center.

$$a_o = \frac{4r}{\sqrt{3}}$$

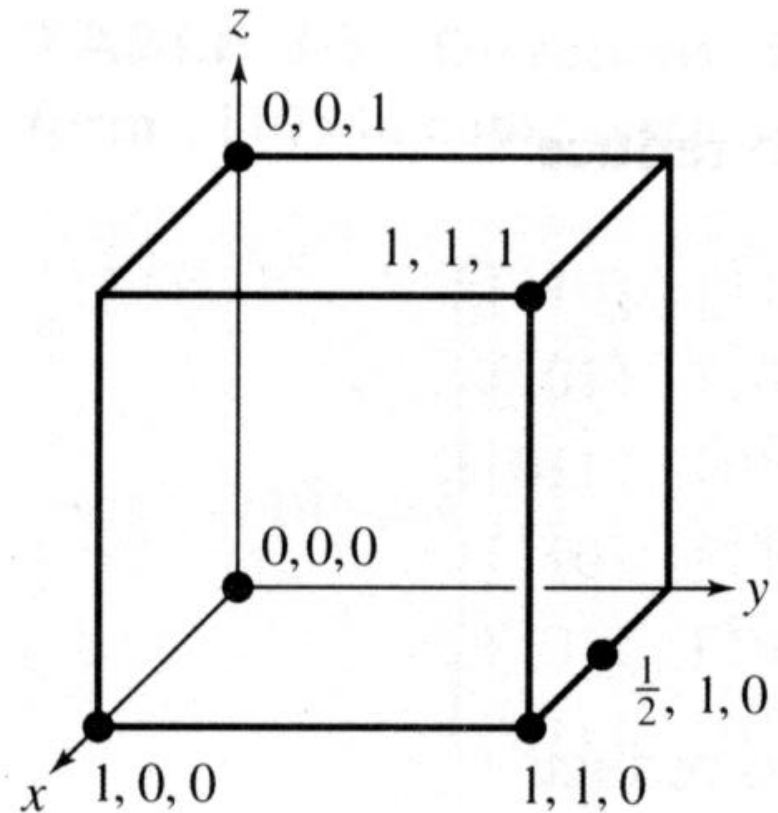
Face Centered Cubic (FCC)



- 4 atoms per unit cell, $6 \frac{1}{2}$ atoms on each face and $8 \frac{1}{8}$ atoms at the corners.
- Close-packed direction $\langle 110 \rangle$, diagonal from opposite corners on a face. $a_o = \frac{4r}{\sqrt{2}}$

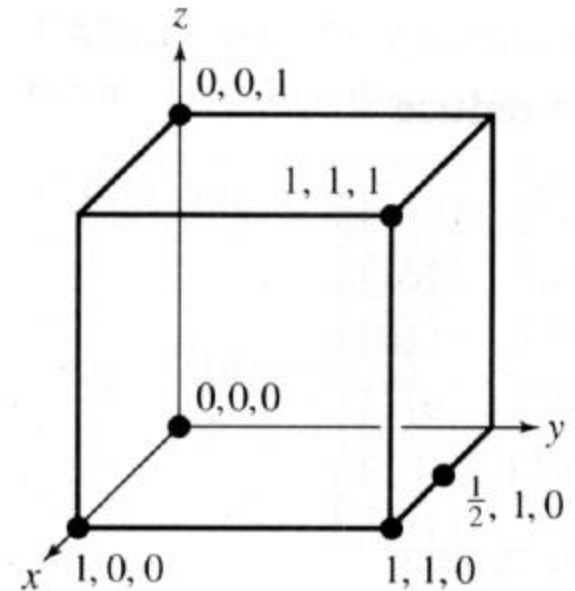
Coordinates of Points

- Use a right-handed coordinate system.
- Written as three distances, with commas separating the numbers (x, y, z).



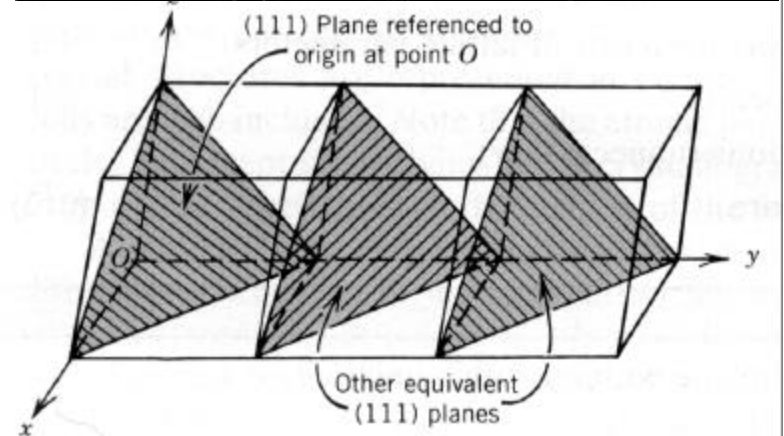
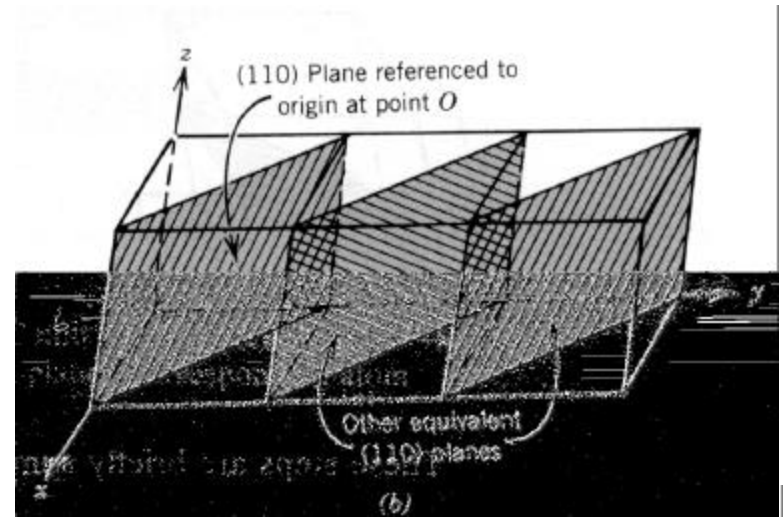
Directions in the Unit Cell

- Miller indices are used to describe the directions.
- **Procedure:** subtract the coordinates of the “tail” from the “head”. Clear fractions and reduce.
- A direction is written as three numbers enclosed in square brackets $[xyz]$, with a line over a number if it is a negative.





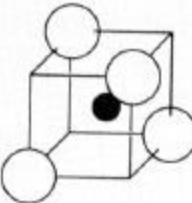

Planes in the Unit Cell

- **Procedures:** identify where the plane intercepts the x , y , and z axis. If it passes through the origin then it must be moved. Take reciprocals of these intercepts. Clear fractions but do not reduce.
- Planes are written as three numbers enclosed in parentheses (xyz). Again with a line over a number if it is a negative



Interstitial Sites

- Interstitial Sites are the small holes between atoms in the crystalline structures.
- Interstitial atoms will only go into interstitial sites that are smaller than they are.

Location of Interstitial	Radius Ratio	Representation
Linear	0–0.155	
Center of triangle	0.155–0.225	
Center of tetrahedron	0.225–0.414	
Center of octahedron	0.414–0.732	
Center of cube	0.732–1.000	