Crystal, Unit Cell, Space Lattice

A unit cell is the most basic and least volume consuming repeating structure of any solid. It is used to visually simplify the crystalline patterns solids arrange themselves in.

A space lattice is an array of points showing how particles (atoms, ions or molecules) are arranged at different sites in three dimensional spaces. Unit cells are easiest to visualize in two dimensions.

CHARACTERISTICS OF A CRYSTAL LATTICE - DEFINITION

1. In a crystal lattice there is the parallelepiped constructed from vectors which correspond to translational periods called unit cells.
2. These can be chosen in different ways. Commonly, unit cells are chosen so that its vertex coincides with one of the atoms of the crystal.
3. Then lattice sites are occupied by atoms, and of the atoms of the crystal.Thus, the lattice sites are occupied by atoms, and vectors that connect the nearest equivalent atoms.
4. The unit cell contains at least one atom of each of the types that make up the crystal.
5. Providing that the unit cell is made up of only one type of atom, it is called monatomic, anymore than that and it is polyatomic. Correspondingly a monatomic lattice is often identified as a simple lattice and a polyatomic one, a composite lattice.

Atomic Packing Factor

•It can be defined as the ratio between the volume of the basic atoms of the unit cell (which represent the volume of all atoms in one unit cell) to the volume of the unit cell it self. APF its depends on the radius of atoms and characterization of chemical bondings .

• It is a dimensionless quantity and always less than unity.

Simple cubic

For a simple cubic packing, the number of atoms per unit cell is one. The side of the unit cell is of length 2*r*, where *r* is the radius of the atom.

$$\mathrm{APF} = \frac{N_{\mathrm{atoms}} V_{\mathrm{atom}}}{V_{\mathrm{unit\ cell}}} = \frac{1 \cdot \frac{4}{3}\pi r^3}{(2r)^3}$$

$$= \frac{\pi}{6} \approx 0.5236$$

Body-centered cubic

The primitive unit cell for the body-centered cubic crystal structure contains several fractions taken from nine atoms one on each corner of the cube and one atom in the center. Because the volume of each of the eight corner atoms is shared between eight adjacent cells, each BCC cell contains the equivalent volume of two atoms

$$\mathrm{APF} = \frac{N_{\mathrm{atoms}} V_{\mathrm{atom}}}{V_{\mathrm{unit\ cell}}} = \frac{2 \cdot \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3}$$

$$= \frac{\pi\sqrt{3}}{8} \approx 0.680\,174\,762\,.$$

Cont…

Hexagonal close-packed

the unit cell is a hexagonal prism containing six atoms. three are the atoms in the middle layer. for the top and bottom layers, the central atom is shared with the adjacent cell, and each of the six atoms at the vertices is shared with other five adjacent cells.

$$\mathrm{APF} = \frac{N_{\mathrm{atoms}} V_{\mathrm{atom}}}{V_{\mathrm{unit\ cell}}} = \frac{6 \cdot \frac{4}{3}\pi r^3}{\frac{3\sqrt{3}}{2} a^2 c}$$

$$= \frac{6 \cdot \frac{4}{3}\pi r^3}{\frac{3\sqrt{3}}{2}(2r)^2 \sqrt{\frac{2}{3}} \cdot 4r} = \frac{6 \cdot \frac{4}{3}\pi r^3}{\frac{3\sqrt{3}}{2} \sqrt{\frac{2}{3}} \cdot 16r^3}$$

$$= \frac{\pi}{\sqrt{18}} = \frac{\pi}{3\sqrt{2}} \approx 0.740\,480\,48\,.$$

Deformation: Overview of deformation behavior and its mechanism

- Deformation in solids is often described as elastic, which is reversible, or plastic, which is non-reversible. In a crystalline solid, the major plastic deformation mechanism is the dislocation movements.
- **Deformation mechanism** refers to the various processes occurring at micro-scale that are responsible for changes in a material 's internal structure, shape and volume.
- Deformation mechanisms is commonly characterized as brittle, ductile and brittle-ductile.
- The driving mechanism responsible is a subject of interplay between internal (composition, grain size and lattice-preferred orientation) and external factors.

Common deformation mechanisms processes subdivisions are:

- Fracturing
- Cataclysmic flow
- Diffusive mass transfer
- Grain boundary sliding
- Dislocation creep
- Dynamic recrystallization

Heat Treatment

Heat treatment involves heating of metal in the solid-state and then subsequently cooled at varied cooling rates. It is very important manufacturing process that can not only help the manufacturing process but can also improve the product, its performance, and its characteristics in many ways. The following changes may be achieved:

- The hardness of Steel may be increased or decreased.
- Internal stresses that are set up due to cold or hot working may be relieved.
- The machinability of Steel may be enhanced.
- The mechanical properties like tensile strength and shock resistance toughness etc may be improved.
- The resistance to corrosion and wear may be increased.
- The cutting properties of the tool may be increased.
- The Grain structure of Steels may be refined.
- The electrical and magnetic properties may be improved.

Annealing

Annealing involves heating the material to a predetermined temperature and hold the material at the temperature and cool the material to the room temperature slowly. The process involves:

•Heating of the material at the elevated temperature

•Holding the material (Soaking) at the temperature for longer time.

•Very slowly cooling the material to the room temperature

purpose

1) Relieve Internal stresses developed during solidification, machining, forging, rolling or welding

2) Improve or restore ductility and toughness

3) Enhance Machinability

4) Eliminate chemical non-uniformity

5) Refrain grain size

6) Reduce the gaseous contents in steel.