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# Material Science

Ref.

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## • Crystal Structures

(Glass → Supercooled Liquid)

1. Material science is basically study of relationship between structure and Properties of Engineering materials.

2. Based on the structure all engineering materials are classified into two basic types: They are Crystalline materials and Amorphous material.

3. Amorphous material which do not exihibits regular, repeated & orderly arrangement of atoms / Ions / molecules
   eg: Waxes, Polymers, Glass, charcoal etc.

4. Crystalline materials are those materials which exibit 3-D, Long range, Periodicity of arrangement of atom, Ions or molecule in the Internal Structure.

| Crystalline Materials | Amorphous materials |
|---|---|
| ↳ Atomic Solids → Metals | Can exist any state |
| ↳ Ionic Solids → Ceramics | Can be converted into Crystalline materials |
| ↳ molecular Solids → Crystalline Polymers | |

Crystalline $\xrightarrow[\text{Cooling}]{\text{fast}}$ Amorphous

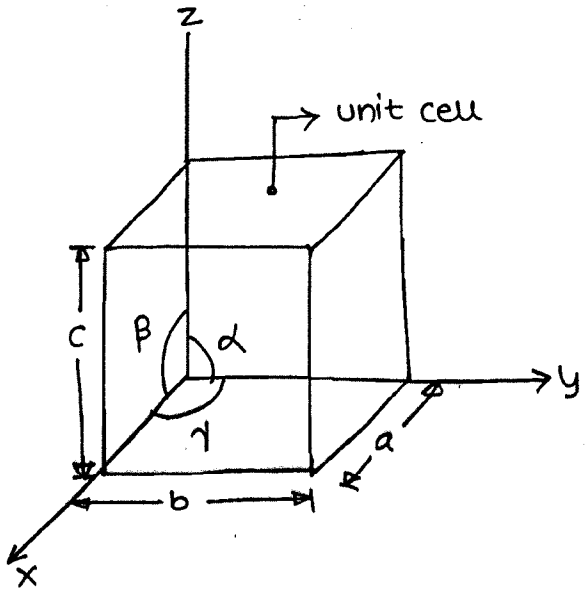
Material type
↳ (We cannot Judge by Naked eye)

5. Crystal structure of unknown material are determine by X-Ray diffraction technique. This is experimental technique.

6. Based on X-Ray diffraction technique all Crystalline materials classified into Seven Crystal System and these are Sub classified into 14 Bravais Lattices

7. The term Crystal System refers to basic shape of unit cell whereas bravais Lattices refers to Atomic Arrangements within a unit cell

8. A unit cell is defined as the smallest representative group of atoms, which when repeated in all the crystallographic direction for Infinite number of times results in the development of crystal lattice.




x, y, z = crystallographic axes

a, b, c = Lattice Parameter

α, β, γ = Interaxial angles

Stability → minimization of Potential energy

| Crystal System | Geometry | Bravais Lattices |
|---|---|---|
| Cubic → Metal | $a=b=c$ $\alpha=\beta=\gamma=90^\circ$ | Simple (S), BCC, FCC |
| Tetragonal | $a=b\neq c$ $\alpha=\beta=\gamma=90^\circ$ | ST, BCT |
| orthoorhombic | $a\neq b\neq c$ $\alpha=\beta=\gamma=90^\circ$ | SO, BCO, FCO ECO |
| Rhombohedral | $a=b=c$ ; $\alpha=\beta=\gamma\neq90^\circ$ | SR |
| Hexagonal For metal | $a=b=c$ $\alpha=\beta=90^\circ, \gamma=120^\circ$ | SH |
| Monoclinic | $a\neq b\neq c$ $\alpha=\gamma=90^\circ\neq\beta$ | SM, ECM |
| Triclinic | $a\neq b\neq c$ $\alpha\neq\beta\neq\gamma\neq90^\circ$ | STr |

Simple (S)
Body centered (BC)
Face centered (FC)
End centered (EC)
→ Generally

- **Some Important definations**

1. Crystal lattice is defined as a 3-D dimensional Network of Lines in Space, It is also known as Line Lattice.

2. Space Lattice is defined as 3-D dimensional Network of Points in Space, It is also known as Point Lattice.

3. Primitive cell is defined as a simple cubic unit cell having atoms only at the corners.

4. Lattice Parameter is defined as the distance b/w centres of neighbouring corner atoms

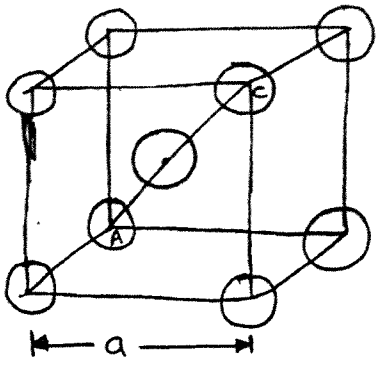
5. Crystal structures characteristics

| Characteristic | BCC | FCC | HCP |
|---|---|---|---|
| a to r relation | $a = \frac{4r}{\sqrt{3}}$ | $a = \frac{4r}{\sqrt{2}}$ | $a = 2r$ |
| Average no of atoms (Nav) | 2 | 4 | 6 |
| Coordination number | 8 | 12 | 12 |
| Atomic Packing Factor (APF) | 0.68 | 0.74 | 0.74 |

Let 'a' = Lattice Parameter

$r$ = Atomic Radius

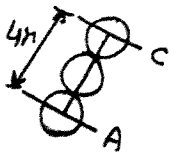
- **BCC**




AC = Body diagonals of Unit cell

$= a\sqrt{3} = 4r$

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

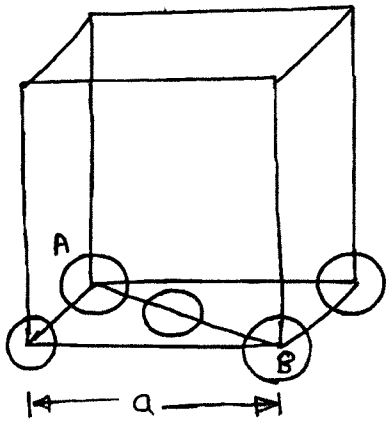



example →

Fe [Except in 910 – 1400°C]

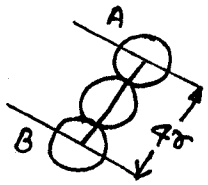
W, Cr, V, Mo, Ta etc.

Hard & Brittle




AB = Face diagonal of unit cell

$= a\sqrt{2} = 4r$




$\therefore \boxed{a = \frac{4r}{\sqrt{2}}}$

Ex. Fe (in 910–1400°C)

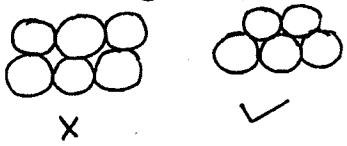
Cu, Al, Ni, Au, Ag, Pt

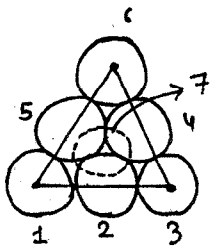
FCC element ⇒ Strong & ductile

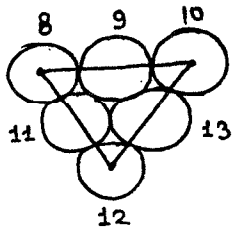
Hence they increase toughness in steel when added as alloying element.

· Stacking Sequence → Sequence of arrangement of atomic Planes, one above the other in order to result in stability to a crystalline structure.

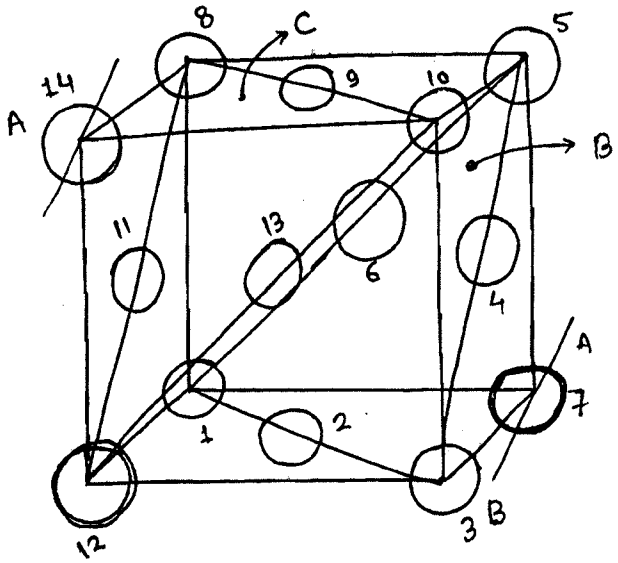
Stability




ABCABCABCABCA---∞




Hardness → Surface

Strength → Volume

Shape, Atomic arrangement, of the atom two orientation