

Study Notes on Solid State

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Solid State

Solids can be classified into **2** based on nature of order in the arrangements of their constituent's particles.

Crystalline solid	Amorphous solid		
1. The constituent particles are arranged in a regular fashion containing short range as well as long range order . The long-range order means the atoms or ions, or molecules are arranged in a regular fashion and this symmetrical arrangement extends throughout the crystal length.	1. The constituent particles are not arranged in any regular fashion. There may be at the most some short-range order only and has a completely random particle arrangements i.e. no regular arrangement, no shape of its own.		
2. They have sharp melting point	2. They melt over a range of temperature.		
3. They are Anisotropic i.e., properties like electrical conductivity, thermal expansion, etc have different values is different direction.	3. They are Isotropic i.e., properties like electrical conductivity, thermal expansion, etc have same value in different directions		
4. They undergo a cleavage. They are considered as True Solid .	4. They undergo an irregular cut. They are also Super cooled Liquid or Pseudo Solid .		
• 5. A B A B A Crystalline solid	5. Amorphous solid		
6. Examples-Quartz, Diamond, NaCl, ZnS, CsCl, Boron Nitride etc.	6. Examples- Glass, Rubber, Plastics etc.		



Unit Cells

Certain properties of a solid which depends only on the constituents of the solid and the pattern of arrangement of these constituents. The smallest amount of the solid whose properties resemble the properties of the entire solid irrespective of the amount taken is called a unit cell. **It is the smallest repeating unit of the solid.** Any amount of the solid can be constructed by simply putting as many unit cells as required.



Unit cells arranged together

In a 3-dimensional space lattice, to specify a unit cell we need the values of <u>three</u> <u>vectors</u> which gives <u>three distances</u> along the <u>three axes</u> and <u>three angles</u> as shown in figure below





PRIMITIVE CUBIC UNIT CELL



In primitive cubic unit cell, the lattice points are corners of the cube. This implies that the atoms are present only at the corners of the cube

Each atom at the corner of the unit cell is shared by eight unit cells. Therefore, the volume occupied by a sphere in a unit cell is just one-eighth of its total volume. Since there are eight such spheres, the total volume occupied by the spheres is one full volume of a sphere. Therefore, a primitive cubic unit cell has effectively one atom.

Packing fraction

It is defined as ratio of the volume occupied by the spheres in a unit cell to the volume of the unit cell

Thus, Void Fraction = (1 – Packing fraction).

Since adjacent atoms touch each other, the edge length of the unit cell 'a' is equal to 2r, where r is the radius of the sphere.

Therefore, Packing fraction (PF) = $\frac{\frac{4}{3}\pi r^3}{(2r)^3} \approx 0.52$. (This implies that 52 % of the volume of a unit

cell is occupied by spheres).

\therefore Void Fraction (VF) \approx 0.48



BODY CENTERED CUBIC UNIT CELL



In body centered cubic unit cell, the lattice points are corners and body center of the cube. That is the atoms are present at all the corners and at the body centered position. Thus, the effective number of atoms in a Body centred Cubic Unit Cell is 2 (One from all the corners and one at the centre of the unit cell).

Since in BCC the body centred atom touches the top four and the bottom four atoms, the length of the body diagonal ($\sqrt{3}a$) is equal to 4r.

The **Packing Fraction** in this case is =
$$\frac{2 \times \frac{4}{3} \pi r^3}{(\frac{4r}{\sqrt{3}})^3} \approx 0.68$$

 \therefore Void fraction (VF) \approx 0.32



FACE CENTERED CUBIC UNIT CELL



In FCC unit cell, the lattice sites are corners and face centers. That is in face centered cubic unit cell, the atoms are present at the corners and the face centers of the cube. <u>The effective number</u> <u>of atoms in FCC is 4 (one from all the corners, 3 from all the six face centres since each face centred atom is shared by two cubes).</u>

Since, each face centred atom touches the four corner atoms, the face diagonal of the cube ($\sqrt{2}$ a) is equal to 4r.

$$\therefore \qquad \text{Packing fraction}(\text{PF}) = \frac{4 \times \frac{4}{3} \pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} \approx 0.74$$

 \therefore Void Fraction (VF) \approx 0.26



HEXAGONAL PRIMITIVE UNIT CELL



A hexagonal primitive unit cell comprises of **3 layers A, B and A** as shown in the figure. Each atom has a **co–ordination number of 12**. Each corner atom is shared by six unit cells, of which three are in the same layer and three are in the upper/lower layer. Thus, each corner atom makes $1/6^{th}$ contribution to a unit cell. There are 12 such corner atoms, so the effective contribution from corner atoms would be $1/6 \times 12 = 2$. There are two atoms at the center of top hexagonal face and the bottom hexagonal face. They would contribute half, as they are shared between two unit cells. Three atoms of B layer are completely inside the unit cell. Thus, <u>the total number of effective atoms in</u>

<u>Hexagonal Primitive unit cell would be</u> $\left(\frac{1}{6} \times 12\right) + \left(\frac{1}{2} \times 2\right) + 3 = 6$

Let ABCD is the base of hexagonal unit cell, AD=AB=a. The sphere in the next layer has its centre F vertically above E it touches the three spheres whose centres are A,B and D.

$$\therefore \qquad \mathsf{AE} = \frac{2}{3} \times \frac{\sqrt{3}}{2} \mathsf{a} = \frac{\mathsf{a}}{\sqrt{3}} = \frac{2\mathsf{r}}{\sqrt{3}}$$

Hence FE =
$$\frac{h}{2} = \sqrt{(2r)^2 - \left(\frac{2r}{\sqrt{3}}\right)^2}$$

 \therefore The height of unit cell (h) = $4r\sqrt{\frac{2}{3}}$

The area of the base is equal to the area of six equilateral triangles, = $6x \frac{\sqrt{3}}{4} (2r)^2$.

The volume of the unit cell = $6 \times \frac{\sqrt{3}}{4} (2r)^2 \times 4r \sqrt{\frac{2}{3}}$.



$$\therefore \qquad \text{Packing fraction (PF)} = \frac{\frac{6 \times \frac{4}{3} \pi r^3}{6 \times \frac{\sqrt{3}}{4} (2r)^2 \times 4r \sqrt{\frac{2}{3}}} \approx 0.74 ;$$

 \therefore Void fraction (VF) \approx 0.26

Density of crystal lattice

The density of crystal lattice is same as the density of the unit cell which is calculated as

ρ=	mass of unit cell	number of effective atoms × mass number	
	volume of unit cell	volume of unit cell × Avogadro number	

 $\rho = \frac{\mathbf{n} \times \mathbf{M}}{\mathbf{N}_{\mathsf{A}} \times \mathbf{V}}$



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