NATIONAL INSTITUTE OF TECHNOLOGY, JAMSHEDPUR

ASSIGNMENT

MATERIAL SCIENCE

ATOMIC PACKING FACTOR

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TOPIC:

ATOMIC PACKING FACTOR

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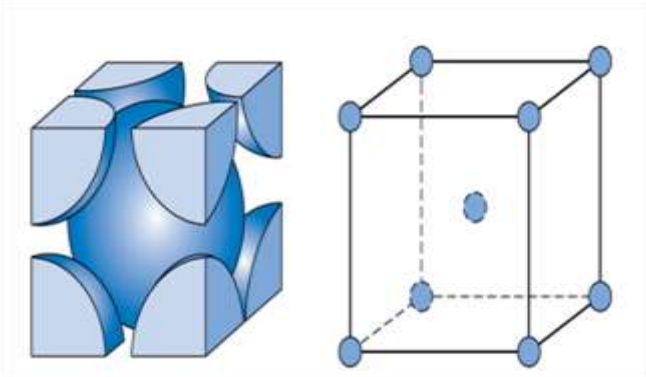

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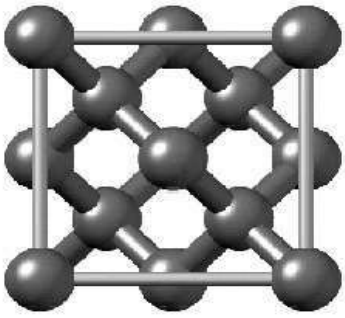


Atomic packing factor:

The packing factor or atomic packing fraction is the fraction of space occupied by atoms, assuming that the atoms are hard spheres.

Expression to calculate packing factor is

$$= \frac{\text{(No. of atoms/unit cell)} \times \text{(volume of each atom)}}{\text{(volume of a unit cell)}}$$

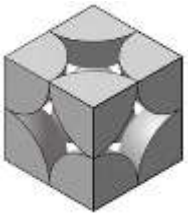
UNIT CELL

- The unit cell is subdivision of a lattice that still retain the overall characteristics of the entire lattice.
- A lattice is a collection of point called lattice point which are arranged in a periodic pattern.

Number of atoms per unit cell

- A specific number of lattice points define each of the unit cell.
- For example the corner of the cell are easily identified as are the body centered and face centered position.

Simple cubic:



- Unit cell of Simple cubic structure has eight corner atoms which are bonded to eight other atoms.
- All sides of cube are equal in length a=b=c
- Here, a=2r
- Volume of a unit cell=$a^3=(2r)^3$
- No. of atoms per unit cell = (1/8)×8 =1
- Atomic Pacing Factor of Simple Cubic

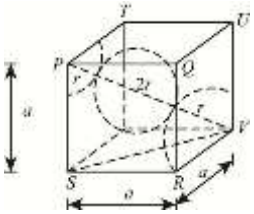
$$= \frac{\text{(No. of atoms/unit cell)} \times \text{(volume of each atom)}}{\text{(volume of a unit cell)}}$$

$$= \frac{1\times(4/3)\times\pi\times r^3}{(2r)^3}$$

$$= 0.52$$

Atomic Packing factor of Simple Cubic = 52%

Body Centered cubic:



- Body centered cubic structure has a unit cell having an atom at its centre and eight atoms at corners.
- Each corner atom is bonded to 8 other atoms and 1 atom is present in the centre.
- As (8x1/8)+1
- So no. of atom in BCC unit cell=2
- $4r=\sqrt{3}a$
- **Examples** of metals with the **bcc** structure are alpha-iron, tungsten, chromium, and beta-titanium.
- The BCC structure has a coordination number of eight.
- Materials having BCC structure are soft and malleable.
- Atomic Packing factor

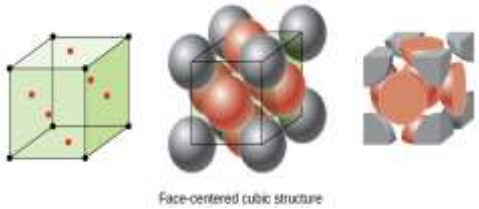
$$= \frac{\text{(No. of atoms/cell)}\times\text{(volume of each atom)}}{\text{(volume of a unit cell)}}$$

$$= \frac{2\times(4/3)\times\pi\times r^3}{(4r/\sqrt{3})^3}$$

= 0.68

Atomic Packing factor of BCC =68 %

Face Centered Cubic:



- A FCC has a unit cell having an atom at the centre of each face of unit cell and 8 corner atoms.
- Each of 8 corner atom contribute 1/8 and each
- face atom contribute 1/2 in each unit cell.
- As (8 x1/8)+((1/2)x 6)=4
- No. of atoms in FCC unit cell=4
- $4r=\sqrt{2}\times a$
- **Examples:** Aluminium and Copper has FCC structure
- The FCC structure has a coordination number of twelve(12).
- FCC structure are usually harder.
- Atomic Packing factor

$$= \frac{\text{(No. of atoms/cell)}\times\text{(volume of each atom)}}{\text{(volume of a unit cell)}}$$

$$= \frac{4\times(4/3)\times\pi\times r^3}{(2\sqrt{2}r)^3}$$

$$= 0.74$$

Atomic Packing factor of FCC=74%

HEXAGONAL CLOSED PACKED:

- Cell of an HCP lattice is visualized as a top and bottom plane of 7 atoms, forming a regular hexagon around a central atom. In between these planes is a half hexagon of 3 atoms.
- There are two lattice parameters in HCP, a and H, representing the basal and height parameters respectively.
- a=2r ; H=4*(√(2/3))r

$$\frac{r}{h} = \cos 30^\circ = \frac{\sqrt{3}}{2}$$

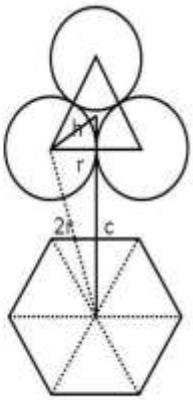
$$h = \frac{2r}{\sqrt{3}}$$

$$(2r)^2 = h^2 + c^2 = \left(\frac{2r}{\sqrt{3}}\right)^2 + c^2$$

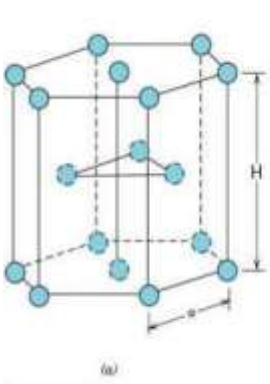
$$c^2 = 4r^2 - \frac{4r^2}{3} = 4r^2 \times \frac{2}{3}$$

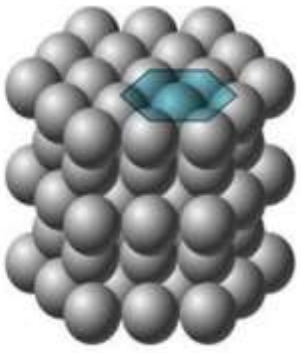
$$c = 2r\sqrt{\frac{2}{3}}$$

$$\text{Height of unit cell} = 2c = 4r\sqrt{\frac{2}{3}}$$



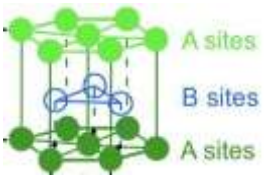
- H/a ratio of 1.633
- No. of atoms per unit cell= (1/6)×12+(½)×2+3=6





- ABAB... Stacking Sequence of HCP

3D Projection 2D Projection



- Co-ordination No. in this structure =12

- **Examples:** Cadmium , Zinc , Titanium are some of the elements with Hexagonal closed packing structure.

- Atomic Packing Factor =

$$\frac{\text{(No. of atoms/unit cell)}\times\text{(volume of each atom)}}{\text{(volume of a unit cell)}}$$

$$= \frac{(6)\times(4/3)\times\pi\times r^3}{6\times\sqrt{3}/4\times a^2 H}$$

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

$$= \pi/\sqrt{18} = 0.74$$

Atomic Packing Factor of HCP=74%

Diamond cubic (D.C.) structure:

- The diamond lattice can be considered to be formed by interpenetrating two FCC lattices along the body diagonal by ¼ cube edge.

- One sub lattice has its origin at the point (0,0,0) and the other at the point quarter of the way along the body diagonal (at the point a/4,a/4,a/4).

- The diamond cubic structure is loosely packed ,since each atom has four nearest neighbor .

NUMBER OF ATOMS PER UNIT CELL

- In the eight corner each atom is shared by eight unit cells

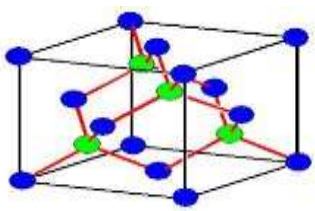
  1/8 *8=1

- The each 6 faces ever single atom which is shared by 2 unit cells

  ½*6=3

- And in every unit cell it has 4 atoms inside 4.

- 1+3+4=8

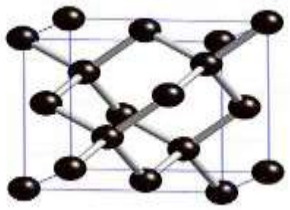


COORDINATION NUMBER

- In a diamond crystal, the carbon atom are linked by the directional covalent bond

- Carbon atoms from covalent bonds with four other carbon atoms that occupy four corners of the cube in a tetrahedral structure.

- In the diamond lattice each atom has four nearest neighbour with which it forms covalent bonds ,thus the coordination number of diamond crystal is 4.



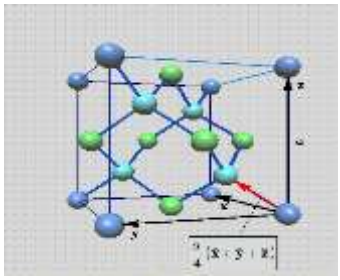
ATOMIC RADIUS

We know that the length of body diagonal in a cube is **√3a.** The atoms present at quarter way along the body diagonal and that at the corners are considered for calculating the relation between radius of atom and edge length of cube. Distance between these atoms is **√3/4*a.**

Therefore, we can notice that

$$2r = \sqrt{3}/4 * a$$

$$\Rightarrow \quad r = \sqrt{3}/8 * a$$



PACKING FACTOR

- Packing factor

  = number of the atoms in the unit cell×volume of one atom/volume of the unit cell

$=8*(4/3*\pi r^3)/a^3$

$=(\pi\sqrt{3})/16$

=0.34

- ***Packing factor =34%***
- Thus it is loosely packed structure
- Example: Carbon ,silicon ,germanium ,and grey tin crystallize in the diamond structure.

CONCLUSION:

Overall, we can notice that the order of atomic packing fraction is as follows:

FCC=Hexagonal>BCC>Simple Cubic>Diamond cubic

Therefore, it can be said that the density of FCC or Hexagonal is maximum while density of diamond is minimum and we can also say that atoms of FCC crystal is more closely packed as compared to other crystal structure.

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