22.3.2012

COORDINATION NUMBER — no. of closest atoms touching an atom

It is the number of atoms touching a particular atom. (in a lattice) Each atom in simple cubic has coordination number = 6

BCC — has 8 for each atom (in BCC no corner atom touches the particular atom but only body atom touches a particular corner atom)

FCC — has 12 (6+6) for each atom.

PACKING FACTOR

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

= fraction of space occupied by atoms per unit cell.

for FCC

$$\text{Packing Factor} = \frac{(4 \text{ atoms/cell})\left(\frac{4}{3}\pi r^3\right)}{a_0^3}$$

$a_0 = 4r/\sqrt{2}$

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

$= 0.74$

BCC packing factor = 0.68

SC = 0.52

$$\text{DENSITY } (\rho) = \frac{(\text{atoms/cell})(\text{atomic mass of each atom})}{}$$

EXAMPLE

Determine the density of BCC iron, which has a lattice parameter of $2.8666\ A^{\circ}$

Atoms/cell = 2

Atomic mass = $55.85\ g/g.mole$

Volume of unit cell = $a_0^3 = (2.866 \times 10^{-8})^3$

$= 23.55 \times 10^{-24}\ cm^3/cell$

Avogadro number = 6.02×10^{23} atoms/g.mole

$$\rho = \frac{2 \times 55.85}{(23.55 \times 10^{-24})(6.02 \times 10^{23})} = 7.879\ Mg\ m^{-3}$$

Allotropic or Polymorphic Transformations

Materials that can have more than one crystal structure are called allotropic or polymorphic.

Iron & Titanium have more than one crystal structures.

At low temp – Iron has BCC

At higher temp – Iron transforms to FCC

These phenomena provide bases for heat treatment.

Characteristics of common Metallic Crystals.

Structure	a_0 versus R	Atoms per Unit Cell	Coordination Number	Packing factor	Typical Metals
Simple Cubic (SC)	$a_0 = 2R$	1	6	0.52	None
Body centered cubic (BCC)	$a_0 = \frac{4R}{\sqrt{3}}$	2	8	0.68	Fe, Ti, W, Mo, Nb, Ta, K, Na, V, Cr, Zr
Face centered cubic	$a_0 = \frac{4R}{\sqrt{2}}$	4	12	0.74	Fe, Cu, Al, Au Ag, Pb, Ni, Pt
Hexagonal close packed	$a_0 = 2R$ $c_0 = 1.633 a_0$	2	12	0.74	Ti, Mg, Zn, Be Co, Zr, Cd.

EXAMPLE

Calculate the change in volume that occurs when BCC iron is heated and changes to FCC iron. At the transformation temperature, the lattice parameter of BCC iron is $2.863\,A^0$ and the lattice parameter of FCC iron is $3.591\,A^0$.

Sol →

Volume of BCC cell $= a^3 = (2.863)^3 = 23.467\,A^3$

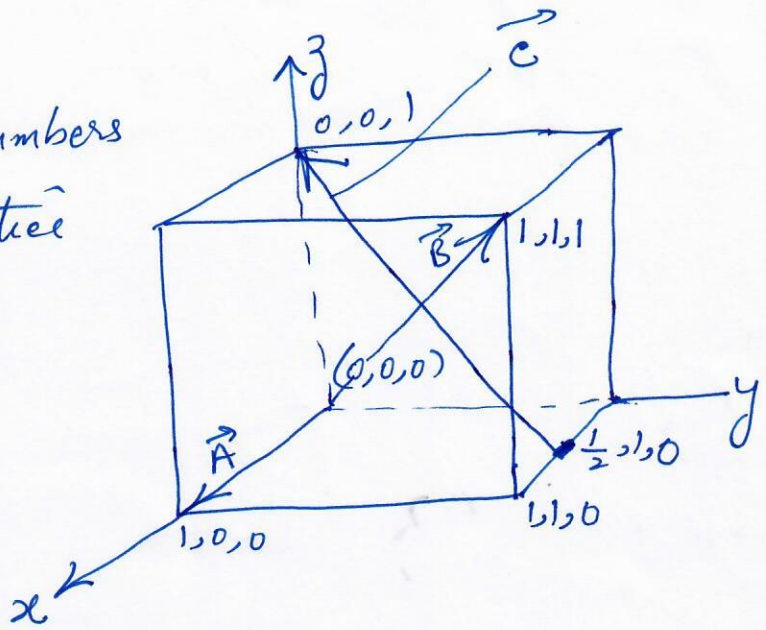
Volume of FCC cell $= a^3 = (3.591)^3 = 46.307\,A^3$

But the FCC unit cell contains 4-atoms and the BCC unit cell contains only 2-atoms

2-BCC unit cells with volume of $2 \times 23.467 = 46.934\,A^3$ will contain 4-atoms

Points, Directions, and Planes in the Unit Cell

Coordinates of Points in the unit cell. The numbers refer to numbers of lattice parameters.



Miller indices => components of vectors

$\frac{y_2 - y}{}$ $(x_2 - x_1)\vec{i} + (y_2 - y_1)\vec{j} + (z_2 - z_1)k$

Miller indices $= [x_2 - x_1, y_2 - y_1, z_2 - z_1]$

$\vec{A} = ((0,0,1) - (\frac{1}{2},1,0)) = [-\frac{1}{2}, -1, 1] = [-1, -2, 2] = [\bar{1}, \bar{2}, 2]$

(Multiply 2 to kill fraction.
