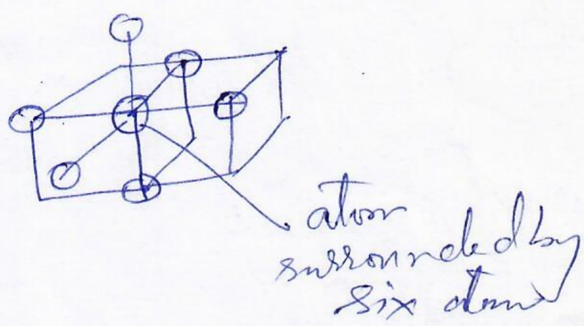
5.4.2012 Interstitial sites

Coordination number

The number of atoms touching a particular atom, or the number of nearest neighbours, is the coordination number and is one indication of how tightly and efficiently atoms are packed together.

In SC coordination number for an atom is six



Example

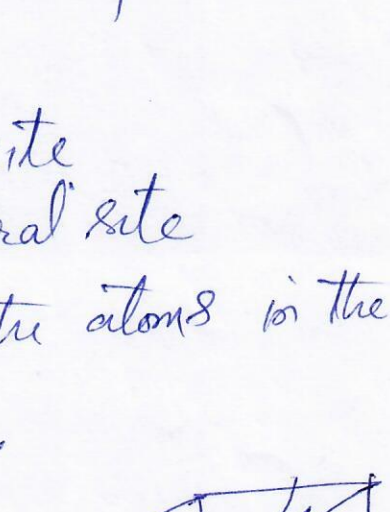
Calculate the radius of an atom that will just fit into

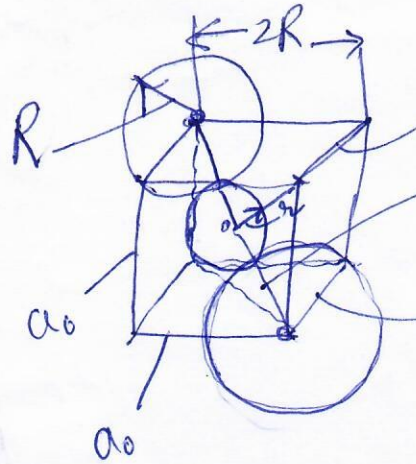
(a) the cubic site

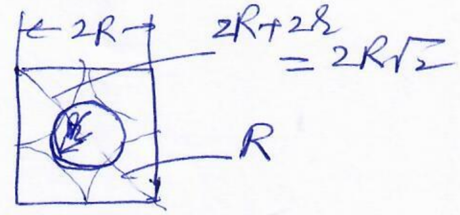
(b) the octahedral site

The radius of the atoms in the normal lattice positions is R.

(a)







$\sqrt{3}a_0 = \sqrt{3} \times \frac{4R}{\sqrt{3}} = 4$

(a) $2R + 2r = 2R\sqrt{3}$

$\frac{r}{R} = 0.732$

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(b) $2R + 2r = 2R\sqrt{2}$

$\frac{r}{R} = 0.414$.

Imperfections in the Atomic Arrangement

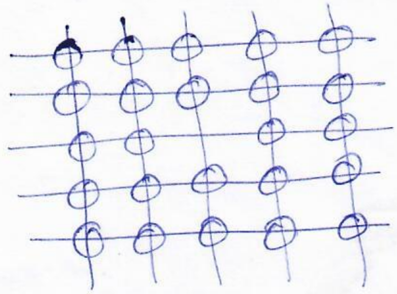
All materials contain imperfections in the arrangement of the atoms which have a profound effect on the behaviour of the material. By controlling these imperfections we create strong materials.

Types of Lattice Imperfections

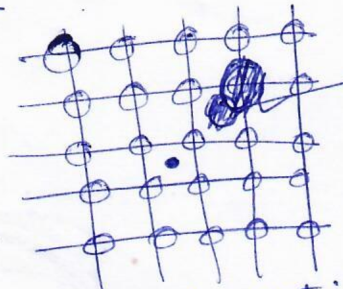
1. Point Defects
2. Line Defects (or Dislocations)
3. Surface Defects

These are all defects in atomic arrangement

Point Defects

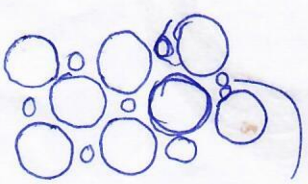


(a) Vacancy

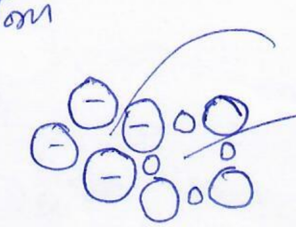


(d) Large Substitutional atom or can be small

(b) Interstitial atom or (c) Substitutional atom



(f) Frankel defect



Schottky defect

All of these defects disrupt the perfect arrangement of surrounding atoms.

(a) Vacancies

A vacancy is produced when an atom is missing from a normal site. Vacancies are introduced into the crystal during solidification. At low temperatures vacancies are low ~~by~~ and vacancies increase with increase in temperature as;

$$n_v = n\, e^{(-Q/RT)}$$

$n_v \longrightarrow$ number of vacancies / cm^3

$n \longrightarrow$ number of lattice point / cm^3

$Q \longrightarrow$ Energy required to produce a vacancy in J/mol

EXAMPLE

Calculate the number of vacancies per cubic centimeter and the number of vacancies per copper atom when copper is at

(a) room temp

(b) 1084°C (just below melting point)

83600 J/mole are required to produce a vacancy in copper.

Sol

a_0 for FCC copper is 3.6151×10^{-8} cm

No. of atoms in 1 cm³ are

$$n = \frac{4 \text{ atoms/cell}}{(3.6151 \times 10^{-8})^3} = 8.47 \times 10^{22} \text{ Copper atom/cm}^3$$

(a) At room temp, $T = 25 + 273 = 298$ °K

$$n_v = (8.47 \times 10^{22})\, e^{\frac{-83,600}{8.31 \times 298}}$$

$$= 1.847 \times 10^{8} \text{ vacancies/cm}^3$$

$$\frac{n_v}{n} = \frac{1.847 \times 10^{8}}{8.47 \times 10^{22}} = 2.18 \times 10^{-15}$$

(b) below melting point $T = 1084 + 273 = 1357$ °K