CRYSTAL PHYSICS

Crystallography Space lattice, Unit Cell & Lattice parameters

Introduction

The matter which surround us is found to exist in three states viz, solids, liquids and gases.

All these materials are composed of atoms and molecules. The constituent particles, atoms or molecules of matter are held together through forces of attraction. *The attractive forces which hold the constituent particles of a substance together are called bonds.*

We know that, some solids are brittle, some are ductile, some are malleable, some are strong, some are weak, some are good conductors of heat and electricity, some are bad conductors of heat and electricity, some are magnetic, some are non-magnetic and so on. The reason for these different properties of the solids is due to their structure. That is, the behavior of the solid materials is closely related to the structure of the material.

Classification of Solids

If we examine the solid materials with which we daily come across, we shall find that most of them do not have any characteristic difference in their outward appearance. But, if we examine them under a microscope we shall find these materials have different internal atomic structures.

Based on the internal atomic structure, the solids can be classified into two categories namely

I. *Crystalline*

II. *Non-crystalline or Amorphous solids.*

Crystalline solids (Crystals)

Crystalline solids or crystals are those, in which the constituent atoms or molecules are arranged in an orderly fashion throughout in a three dimensional pattern.

Each atom or molecule is fixed at a definite point in space at a definite distance from and in a definite angular orientation to all other atoms or molecules surrounding it. Therefore, crystalline solids have well defined geometrical form (pattern), i.e., they have well defined faces and angles between them. Further when crystal breaks, the broken pieces are all having regular shape. *The crystalline solids have directional properties and therefore they are called anisotropic substances.* A crystalline material may be either in the form of a single crystal, (where the solid contains only one crystal) or an aggregate of many small crystals or grains separated by well defined grain boundaries also known as *polycrystalline solid.*

Few examples for crystalline solids: **Copper, silver, Aluminium, iron** etc.

Crystallography: *The study of the geometric form and other physical properties of crystalline solids by using X-rays, electron beams and neutron beams etc., is termed as the science of crystallography.*

Examples for single crystals: ***Sugar, common salt (NaCl), diamond*** *etc. These single crystals are produced artificially from their vapour or liquid state.*

Amorphous solids (Non-crystalline solids)

"Amorphous" means "without form".

In amorphous solids, the constituent particles, atoms or molecules are not arranged in an orderly fashion, i.e., the same atomic groups are arranged more randomly.

These solids have no directional properties and therefore they are called isotropic substances. These amorphous solids do not have a sharp melting point.

Examples: Plastics, rubber and glass.

Note:

Super cooled liquids

The materials like glass, which exhibit some of the properties of a solid like hardness, definite shape etc., but are not crystalline, are regarded as super cooled liquids.

Fig.1

Difference between crystalline and non-crystalline material

Sr. No.	Crystalline material	Non-crystalline material
1	They have definite and regular geometrical shapes which extend throughout the crystal.	They do not have definite geometrical shape.
2	They are anisotropic.	They are isotropic.
3	They are most stable.	They are less stable.
4	They have sharp melting point. Examples: Diamond, NaCl, KC1	They do not have sharp melting point. Examples: Glasses, plastics, rubber

Crystal Structure

The crystal structure gives the arrangement and disposition of atoms within a crystal. *Determination of crystal structure with the help of X-rays is known as X-ray crystallography.* X-rays are most widely used to study the crystal structure because the wavelength of X-rays (10^{-12} to 10^{-10} m) is most comparable with the inter-atomic distances.

Fundamental crystallographic terms (definitions)

a) Lattice

Lattice is defined as an array of points such that every lattice point has got the same environment or every point is indistinguishable from the other lattice point. It is an imaginary concept.

b) Space lattice or crystal lattice

Definition - 1: *A three dimensional collection of points in space is called a space lattice or crystal lattice. The environment about any particular point is in every way the same.* That is, space lattice is an idealized geometrical (imaginary) concept by which crystal structures can be described.

Figure 2

Figure 3

c) Lattice points

Lattice points denote the position of atoms or molecules in the crystal.

d) Basis or Motif

A crystal structure is formed by associating with every lattice point a unit assembly of atoms or molecules (i.e., one or more atoms or molecules) identical in composition, arrangement and orientation. This unit assembly is called the basis or pattern or motif. The logical relation is

Space lattice + Basis = Crystal structure.

(a) Lattice (b) Basis (c) Lattice + Basis

Fig.4.

The number of atoms in the basis may be as low as one. Examples are Aluminium and Barium. In NaCl and KCl the basis is two atoms and in CaF_2 the basis is three atoms. But, there are structures for which the basis exceeds 1000 atoms.

***Note**: A crystal lattice refers to the geometry of a set of points in space. The crystal structure refers to the actual arrangement of atoms or molecules in the space.*

e) Lattice planes

A set of parallel and equally spaced planes in a space lattice which include all lattice points are called as lattice planes.

The different ways of drawing the lattice planes for the array of figure 3 are shown in figure 5.

Fig 5

f) **Unit cell:** The unit cell is the smallest block or geometric figure from which the entire crystal is built up by repetition in three dimensions.

- *The unit cell may be considered as the brick of a wall where the latter represents the crystal. We know that, the shape of the wall depends upon the shape and arrangement of the brick. Similarly the shape of the crystal will depend upon the shape of the unit cell and the arrangement of atoms within the unit cell.*
- *Translation: Motion of a body in which all the points in the body follow parallel paths.*
- *Other terms used to represent a unit cell: The unit cell is also known as basic cell or basic unit or fundamental unit or fundamental elementary pattern or building block or lattice unit.*

g) Lattice parameters

Fig. 6. Lattice Parameters

The figure 6 shows a unit cell of a three dimensional crystal lattice. *The lines drawn parallel to the lines of intersection of any three faces of the unit cell which do not lie in the same plane are called crystallographic axes.* The intercepts *a, b* and *c* are nothing but the edges of the unit cell, (i.e., the distance between two lattice points) which defines the dimensions of a unit cell. *These intercepts are known as its primitives or characteristic intercepts along the axes.* These three quantities *a, b* and c are also *called the fundamental translational vectors.* The angles between *(a, b), (b, c)* and *(c, a)* are denoted by γ, α and β respectively.

The three angles (α, β and γ) are called interfacial angles. Both, the intercepts and interfacial angles constitute the lattice parameters of the unit cell.

The form and actual size of the unit cell can be determined if the values of intercepts and interfacial angles are known.

h) Primitive cell P

A primitive cell is the simplest type of unit cell which contains one lattice point per unit cell (contains lattice points at its corner only).

Example: Cubic cell.

If there is more than one lattice point it is called a non-primitive cell.

Example: BCC and FCC contain more than one lattice point per unit cell.

If the number of lattice points per unit cell is two (BCC), three and four (FCC) the unit cell is called doubly primitive, triply primitive and quadruple primitive respectively.

Multiple Choice Questions

Q.1 A crystal Lattice refers to the geometry of a set of-----

a) Points in Space

b) Atoms in Space

c) Molecules in Space

d) Elements In space

Q.2 A unit Assembly of atoms or molecules identical in composition is called as-

a) Basis

b) Unit cell

c) Lattice

d) N

Bravais lattices, Cubic systems: SC, BCC & FCC

Crystal System

On the basis of the lengths and directions of the axes of the symmetry, all the crystals may be classified into seven systems.

The shapes of the unit cells are shown in Fig. Of these seven crystal systems, the cubic system is the simplest and most symmetrical in which $a = b = c$ and $\alpha = \beta = \gamma = 90°$. It is interesting to note that more than half of the naturally occurring crystals belong to the cubic system.

According to the different values of the lattice parameter, seven crystal systems can be formed as follows:

S. No.	Crystal System	Basic Vectors	Interfacial Angles
1.	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$
2.	Monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90° \neq \gamma$
3.	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$
4.	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$
5.	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$
6.	Rhombohedral (trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$
7.	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$

Bravais Space Lattice:

In 1845, Bravais showed that there are only 14 ways of arranging points in space so that the environment looks the same from each point. These 14 lattices are called Bravais space lattices, each of which has the same collection of symmetry elements at the lattice points. They are shown below

Fig.7. Bravais Lattices

For cubic system, three types of Bravais lattices are possible, viz.:

(i) Simple cubic (SC) (e.g. Palladium)

(ii) Body-centered cubic (BCC) (e.g. Molybdenum)

(iii) Face-centered cubic (FCC) (e.g. Ni, Cu, NaCl)

Some Important terms:

1. **Number of atoms per unit cell or Effective number**

   The total number of atoms present in a unit cell is known as number of atoms per unit cell.

2. **Co-ordination number**

   Co-ordination number is the number of nearest neighbours directly surrounding a given atom.

3. **Atomic radius**

   It is defined as half of the distance between to nearest neighbours in a crystal of a pure element.

   It is usually expressed in terms of cube edge ***a.*** Any two nearest neighbouring atoms touch each other.

4. **Atomic packing factor (Packing density or Density of packing)**

   It is defined as the ratio of the volume of atoms per unit cell to the total volume occupied by the unit cell.

5. **Voids:**

The space in the unit cell which is left unoccupied by atoms is called as the void

$$\text{void} = (100 - \text{APF in } \%)$$

(a) Simple Cubic Structure:

Fig.8

In simple cubic crystal structure the atoms or molecules are located at the each corner of the cube or the unit cell. Thus there is only one basis atom per unit cell. As it is the cubic crystal structure the lattice constants along the crystallographic axes are equal.

Thus we have $\boldsymbol{a = b = c}$

Also as the for the cubic structure one should have

$\boldsymbol{\alpha = \beta = \gamma = 90^0}$

i. Number of atoms per unit cell:

Fig.9

The figure 9 shows the unit cell of a simple cubic structure. In this case, there are only 8 atoms, one at each corner of the cube or the unit cell. In actual crystals, each and every corner atom is shared by 8 adjacent unit cells. Therefore, each and every corner atom contributes 1 / 8th of its part to one unit cell. Total number of corner atoms $N_c = 8$

∴ The total share of the entire corner atoms/unit cell = 8 × 1 / 8 = 1.

∴ Number of atoms/unit cell = 1

In other words, the effective number of lattice points in a simple cubic structure is one. Thus, simple cubic is a primitive cell.

ii. Co-ordination Number:

Coordination number = 6

Fig.10

Simple cubic unit cell consists of 8 comer atoms. Let us consider any one corner atom as shown in figure 10. For the atom at the centre there are 4 nearest neighbours in its own plane (horizontal plane) and there are 2 more nearest atoms, one directly above and the other one directly below. Except these six atoms all the other atoms lie at greater distances from it. Thus, the coordination number for an atom in simple cubic is 6.

iii. Relation between 'a' and 'r':

Let us consider one face of the simple cubic structure, figure 11. In this structure the atoms touch each other along the edges.

Fig.11: Simple cubic structure

Hence, the nearest neighbour distance is 2r = ***a.*** Therefore, r = ***a/2.***

iv. Atomic Packing Factor (APF):

The packing factor or packing density of the simple cubic structure can be calculated as follows:

$$\text{APF} = \frac{\text{No. of atoms per unit cell x Volume of one atom}}{\text{Volume of the unit cell}}$$

In simple cubic,

The number of atoms per unit cell = 1

Volume of one atom= $\frac{4}{3}\pi r^3 = \frac{4}{3}\pi\left[\frac{a}{2}\right]^3 \left[\because r = \frac{a}{2}\right]$

Volume of the unit cell = a^3

$$\text{APF} = \frac{1 \times \frac{4}{3}\pi\left[\frac{a}{2}\right]^3}{a^3}$$

$$\text{APF} = \frac{\pi}{6} = 0.52$$

52 % of the volume is occupied by atoms and remaining 48 % volume is vacant.

v. Void:

The space in the unit cell which is **left unoccupied** by atoms is called as the void

$$\textbf{void} = (100 - \text{APF in } \%)$$

$$void = (100 - 52) = 48\ \%$$

(b) Body Centered Cubic Structure

Fig. 12

In body centered cubic structure, there are 8 atoms at each corner of the unit cell plus one atom at the geometric centre of the unit cell. Thus the corner atom touches the body central atom through the body diagonals. In this way there are two basis atoms, one located at the corner & the other one at the center of the body.

i. Number of Atoms Per Unit Cell:

Fig. 13

In this case, there are 8 atoms one at each corner of the unit cell plus one atom at the centre of the unit cell, figure 10. Each and every corner atom is shared by 8 adjacent unit cells. The atom at the body centre is not shared by any other unit cell. Number of unshared atoms/unit cell = 1.

The total share of all the corner atoms per unit cell is 8 x 1 / 8= 1.

Hence, total number of atoms/unit cell = 1 + 1 = 2

ii. Co-ordination Number:

In this structure, there will be one atom at the body centre and eight atoms at the 8 corners of the unit cell figure 14. Thus, for an atom at the body centre obviously, there are 8 nearest neighbours (corner atoms). Hence, the co-ordination number of an atom in body centered cubic structure is 8. The corner atoms do not touch each other. But, each corner atom touches the body centre along the body diagonal.

Coordination number = 8

Fig. 14

Alternative method

The coordination number can also be determined in another way as follows.

We know that in a BCC structure, each corner atom is surrounded by eight ether body centered unit cells. Therefore, the nearest adjacent neighbours are the body centered atoms of the eight surrounding unit cells. Thus, the coordination number is 8.

ii. Relation between 'a' and 'r':

ii. Relation between 'a' and 'r':

Fig.15: Body Centered Cubic structure

In this structure, the corner atoms do not touch each other. But, each corner atom touches the body centered atom along the body diagonal, figure 15. Thus, the diagonal of the cube AD is 4r. But, from the geometry of the cube,

$$(AD)^2 = (AC)^2 + (CD)^2 = (AB)^2 + (BC)^2 + (CD)^2 \; [\because (AC)^2 = (AB)^2 + (BC)^2]$$

$$(AD)^2 = a^2 + a^2 + a^2 = 3a^2 \; [\because AB = BC = CD = a]$$

$$AD = a\sqrt{3}\,; But\ AD = 4r$$

$$\therefore 4r = a\sqrt{3} \quad \text{OR} \quad r = a\frac{\sqrt{3}}{4}$$

iii. Atomic Packing Factor (APF):

The packing factor or packing density of the body centered cubic structure can be calculated as follows:

$$\text{APF} = \frac{\text{No. of atoms per unit cell} \times \text{Volume of one atom}}{\text{Volume of the unit cell}}$$

The no of atoms per unit cell = 2

$$\therefore \text{Volume of 2 atoms} = 2 \times \frac{4}{3}\pi r^3 = \frac{8\pi}{3}\left[\frac{a\sqrt{3}}{4}\right]^3 = \pi a^3 \frac{\sqrt{3}}{8} \quad \left[\because r = a\frac{\sqrt{3}}{4}\right]$$

Volume of the unit cell = a^3

$$\text{APF} = \frac{\pi a^3 \frac{\sqrt{3}}{8}}{a^3}$$

$\therefore$ APF = 0.68

$\therefore$ 68% of the volume is occupied by atoms and remaining 32 % volume is vacant.

iv. Void:

The space in the unit cell which is **left unoccupied** by atoms is called as the void

$$\textbf{void} = (100 - \text{APF in } \%)$$

$$void = (100 - 68) = 32\ \%$$

(c) Face Centered Cubic Structure

Fig.16

In face centered cubic structure, there are 8 atoms at each corner of the unit cell. Also we have in addition one atom at the center of the each face of the cube. Thus the corner atom touches the face central atom along the face diagonals. In this way there are two basis atoms, one located at the corner & the other one at the center of the face.

i. Number of atoms per unit cell:

Fig.17

In this case, there are 8 atoms, one at each corner of the unit cell and six atoms at the centers of six faces of unit cell figure 17.The total share of all the corner atoms per unit cell is 8x1/8=1.

Now, consider the atoms at the face centre of the unit cell. Each such atom is shared by only two unit cells, which lie on either side of the plane in which the atom is located. The total share of all the face centered atoms per unit cell = 6 x 1/2 = 3. Hence, the total number of atoms/unit cell is 1 + 3 = 4.

ii. Co-ordination Number:

Coordination number = 12

Fig.18

In this system, there are 8 corner atoms and six face centered atoms one at the centre of each face. To calculate the coordination number, consider any corner atom (the blue coloured one at the center). In its own plane it has 4 face centered atoms as nearest neighbour. In a plane which lie just above this corner atom, it has 4 more face centre atoms as nearest neighbors' and similarly, in a plane which lie just below this corner atom it has 4 more face centered atoms as nearest neighbours. The total number of nearest atoms to any corner atoms is 4 + 4 + 4 = 12. Hence, the coordination number is 12.

iii. Relation between 'a' and 'r':

Fig.19: Face Centered Cubic structure

In face-centered cubic structure, the atoms touch each other along the diagonal of any face of the cube. The diagonal of the cube AC is 4r.

But, from the geometry of the figure

$(AC)^2 = (AB)^2 + (BC)^2 = a^2 + a^2 = 2a^2$

$\therefore AC = a\sqrt{2}$ $\quad [\because AC = 4r]$

$4r = a\sqrt{2}$

Hence $\quad r = a\frac{\sqrt{2}}{4}$

iv. Atomic Packing Factor (APF):

The packing factor or packing density of the face centered cubic structure can be calculated as follows:

$$APF = \frac{No.\ of\ atoms\ per\ unit\ cell \times Volume\ of\ one\ atom}{Volume\ of\ the\ unit\ cell}$$

The no of atoms per unit cell $= 4$

$$\therefore \text{Volume of 4 atoms} = 4 \times \frac{4}{3}\pi r^3 = \frac{16\pi}{3}\left[\frac{a\sqrt{2}}{4}\right]^3 = \pi a^3 \frac{\sqrt{2}}{6} \quad \left[\because r = a\frac{\sqrt{2}}{4}\right]$$

Volume of the unit cell = a^3

$$APF = \frac{\pi a^3 \frac{\sqrt{2}}{6}}{a^3} = \pi \frac{\sqrt{2}}{6}$$

$$\therefore APF = 0.74$$

$\therefore$ 74% of the volume is occupied by atoms and remaining 26 % volume is vacant

v. Void:

The space in the unit cell which is left **unocc**upied by atoms is called as the void

$$\textbf{void} = (100 - \text{APF in } \%)$$

$$void = (100 - 74) = 26\ \%$$

Relation between Lattice Constant and Density

Consider a cubic crystal.

Let, the lattice constant of the cell = a

The number of atoms per unit cell = n

The atomic weight of the crystalline substance or compound = A

The density of the unit cell =ρ

The Avogadro's number = N

[Avogadro's number gives the number of molecules per kilogram mole of the substance]

∴ Mass of each Atom = $\frac{A}{N}$

Hence, Mass of n Atoms (i.e., mass in each unit cell)= $\frac{A}{N}n$

∴ Density of a unit cell is

$$\rho = \frac{\text{Mass of a unit cell}}{\text{Volume of a unit cell}}$$

$$\rho = \frac{A \times n}{Na^3}$$

$$a^3 = \frac{An}{N\rho}$$

$$a^3 = \frac{Atomic\ weight \times Number\ of\ atoms\ per\ unit\ cell}{Avagadro\ Number \times Density}$$

Hence, using the above equation, we can calculate the lattice constant '**a**'.

ELECTRICAL PROPERTIES

Introduction

The objective of this chapter is to explore the electrical properties of materials, i.e. their responses to an applied electric field. We begin with the phenomenon of electrical conduction: the parameters by which it is expressed, the mechanism of conduction by electrons, and how the electron energy band structure of a material influences its ability to conduct. These principles are extended to metals, semiconductors and insulators. Particular attention is given to the dielectric characteristics of insulating materials. The final sections are devoted to the peculiar phenomena of Ferro electricity and piezoelectricity.

The electrical conductivity is one of the properties of materials that vary most widely and the best conductors such as copper and silver have values of about $10^{8}\Omega^{-1}m^{-1}$ and a good insulator such as polystyrene has conductivity $10^{-15}\Omega^{-1}m^{-1}$. In a metal, the current is carried by conduction electrons, and hence the name *electronic conduction*.

30 Minutes

ENERGY BAND STRUCTURES IN SOLIDS (Board Teaching & PPT)

In an isolated atom electron occupy well defined energy states, when atoms come together to form a solid, their valence electrons interact with each other and with nuclei due to Coulomb forces. Inter atomic spacing is small in solids compared with liquids and gases. Due to this closeness of atoms, energy levels of the atoms are disturbed. Energy levels of the valence electrons are most affected. Each energy level splits up into a number of closely spaced levels. These split energy levels form a continuous band called energy band as shown in fig 3.13.

Energy level is the discrete energy of an electron in an atom. But energy band is the energy of the same electron when it is in a solid. At large separation distances, each atom is independent of all the others, so they have energy levels. But the atoms come close to each other, electrons respond to the influence of other nuclei and electrons. So each atomic level splits into N levels each of which may be occupied by pairs of electrons of opposite spins. The extent of splitting depends on inter atomic separation.

Firstly outer most electron shells are disturbed.

In each energy band, energy levels are discrete; the difference between adjacent states is infinitesimally small. At the equilibrium spacing, band formation may not occur for electron sub shells nearestthe nucleus as shown in fig 3.13. Further gaps exist between adjacent bands. The electron does not have any energy with in energy gap.

Figure 3.13: Electron energy versus inter atomic separation for an aggregate of atoms

ENERGY BAND STRUCTURES AND CONDUCTIVITY

There are four types of band structures which are possible at 0 K. The highest filled state at 0 K is called Fermi Energy (E_F). The two important energy bands are:

Valence band: Valence band is the wide range of energies possessed by the valence electrons.The highest filled energy band where the electrons are present at 0 K.

Conduction band: Conduction band is the wide range of energies possessed by the conduction electrons. A partially filled or empty energy band where the electrons can increase their energies by going to higher energy levels within the band when an electric field is applied.

Energy Band Structures and Conductivity for metals

In metals (conductors), highest occupied band is partially filled or bands overlap. Conduction occurs by promoting electrons into conducting states that starts right above the Fermi level. The conducting states are separated from the valence band by an infinitesimal amount. Energy provided by an electric field is

sufficient to excite many electrons into conducting states.

Ex: Copper atomic number is 29, its electronic configuration is - $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$. Each copper atom has one 4s electron. For a solid consisting of N atoms, the 4s band can accommodate 2N electrons. Thus only half of the 4s band states are filled. This is shown in fig 3.14(a).

For the second band structure, there is an overlap of filled band (valence band) and empty band (conduction band). Ex: Magnesium atomic number is 12, its electronic configuration is $1s^2 2s^2 2p^6 3s^2$. Each magnesium atom has two 3s electrons. In a solid of magnesium, the 3s and 3p bands are overlapped. This is shown in fig 3.14(b).

Figure 18.4 The various possible electron band structures in solids at 0 K. (*a*) The electron band structure found in metals such as copper, in which there are available electron states above and adjacent to filled states, in the same band. (*b*) The electron band structure of metals such as magnesium, wherein there is an overlap of filled and empty outer bands. (*c*) The electron band structure characteristic of insulators; the filled valence band is separated from the empty conduction band by a relatively large band gap (>2 eV). (*d*) The electron band structure found in the semiconductors, which is the same as for insulators except that the band gap is relatively narrow (<2 eV).

Figure 3.14: The various possible electron band structures in solids at 0 K. (a) The electron band structure found in metals such as copper, in which there are available electron states above and adjacent to filled states, in the same band. (b) The electron band structure of metals such as magnesium, wherein there is an overlap of filled and empty outer bands. (c) The band structures of insulators. (d) The band structure of semiconductors.

Energy Band Structures and Conductivity for Semiconductors and insulators:

As shown in fig 3.14, (c) and (d) band structures are similar. The valence band is completely filled with electrons. There is large energy gap between filled valence band and empty conduction band. Ex: Insulators. If the energy gap between valence and conduction band is small than i.e. semiconductor. Electrical conduction requires that electrons be able to gain energy in an electric field. To become free, electrons must be promoted (excited) across the band gap. The excitation energy can be provided by heat or light. In semiconductors and insulators, electrons have to jump across the band gap into conduction band to find conducting states above E_f.The energy needed for the jump may come from heat or from irradiation at sufficiently small wavelength (photo excitation).

The difference between semiconductors and insulators is that in semiconductors electrons can reach the

conduction band at ordinary temperatures, where in insulators they cannot. An electron promoted into the conduction band leaves a hole(positive charge) in the valence band, that can also participate in conduction. Holes exist in metals as well, but are more important in semiconductors and insulators.

10 Minutes

Verify

1. In terms of electron energy band structure, discuss reasons for the difference in electrical conductivity between metals, semiconductors, and insulators.
2. Explain formation of energy band structure considering decrease in inter atomic spacing in to account.
3. Define equilibrium spacing.

Session 11

Process of electrical conduction in metals, conductivity, mobility and Matthiessen's rule

30 Minutes

Process of electrical conductivity in metals (Board Teaching)

It is defined as the voltage apply to a conductor which is equal to the product of current passing through the conductor times its resistance. This law is independent of size and shape of the conductor under consideration. However, it can alsobe expressed in terms of current density J and electric field E. The current density in the direction of electric field is defined as the amount of charge flowing across a unit area of cross section per unit time in a conductor. If *n* is a number of electrons crossing a unit area in unit time then the amount of charge is equal to "– ne". Average velocity of electrons is the drift velocity. The flow of charge per unit time through unit area of the conductor is equal to the product of electon charge times the drift velocity of the electrons which is current density

$$J = -nev_d.$$

$$J = \frac{ne^2\tau}{m} E$$

Or

$$J = \sigma E$$

It follows that the electric current density is proportional to the applied electric field. This equation is known as Ohm's law and proportionality constant is called electrical conductivity σ.

(iv) Electrical conductivity

In general the electrical conductivity is a property of a conducting material which allows the flow of current.

$$\sigma = \frac{ne^2\tau}{m}$$

This is one of the central results of the classical free electron theory of metals. This formula is not useful for calculating the conductivity of a given metal, since it contains an unknown term called relaxation time. The theory itself has important implications. This picture of electron gas undergoing constant scattering and is still used. For a particular metal *n*, *e* and *m* are constants. Therefore, the electrical conductivity depends on the relaxation time 'τ'. Thus in the absence of collision process the relaxation time is infinite and hence the conductivity becomes infinite. The electrical conductivity can also be expresses in terms of mobility.

$$\sigma = ne\mu$$

Thus in general the electrical conductivity of a metal depends on two factors. They are n and μ.

(v) Electrical Resistivity (ρ)

Electrical resistivity is a measure of how strongly a materialopposes the flow of electric current. A low resistivity indicates a material that readily allows the movement of electric charge. The S.I. unit of electrical resistivity is Ω-m. It is commonly represented by a Greek letter ρ.

(vi) Electrical conductivity (σ)

It is the ability of a substance to conduct an electric current. It is the inverse of the resistivity.

Ohms law

Ohm's law can be rewritten in terms of the current density J = I/A as: J = σ E. Ohm's law can be expressed in both microscopic and macroscopic forms.

(Macroscopic form)

(Microscopic form)

Electrical conductivity varies between different materials by over 27 orders of magnitude.

Metals: $\sigma > 10^5\ (\Omega.m)^{-1}$

Semiconductors: $10^{-6} < \sigma < 10^5\ (\Omega.m)^{-1}$

Insulators: $10^{-6}\ (\Omega.m)^{-1} < \sigma < 10^{-20} (\Omega.m)^{-1}$

One of the best materials for electrical conduction (low resistivity) is silver, but its use is restricted due to the high cost. Most widely used conductor is copper: inexpensive, abundant, high σ, but rather soft – cannot be used in applications where mechanical strength is important.

Metal	*Electrical Conductivity* $[(\Omega\text{-}m)^{-1}]$
Silver	6.8×10^7
Copper	6.0×10^7
Gold	4.3×10^7
Aluminum	3.8×10^7
Iron	1.0×10^7
Brass (70 Cu–30 Zn)	1.6×10^7
Platinum	0.94×10^7
Plain carbon steel	0.6×10^7

Table 3.1: Room temperature electrical conductivities for eight common metals and alloys

Solid solution alloying and cold working improve strength but decrease conductivity. If hardeningis preferred, Cu-Be alloy is used. When weight is important one uses aluminum, which is half as good as Cu and more resistant to corrosion. Heating elements require low (high R), and resistance to high temperature oxidation: nickel chromium alloy.

Drift velocity of electrons :

When an electric field E is applied to a conductor, the electrons modify their random motion and move with an average drift velocity v_d in a direction opposite to that of the electric field and an electric current is established in the conductor. The flow of current in a conductor is an indication that the electron in it moves in a specific direction. As a result, Maxwell-Boltzmann distribution function of the electrons in the conductor undergoes a change. The directional motion of the electrons is due to the applied electric field. The group of electrons within the conductor drifts in the direction opposite to the applied electric field. This motion is called a drift motion and the associated velocity of the electron is called drift velocity.

Due to the electric field E an electron inside the metal experiences a force and this force F is equal to the product of electric charge and electric field.

$$F=-e * E$$

where'–e' is the charge of the electron. As a result, the electron acquires acceleration. According to newtons second law of motion, the force experienced by the electron is given by

$$F=m * a$$

where'a' is the acceleration of the electron and m is the mass of the electron. Eliminating F from the above equations gives the acceleration of the electron under the influence of electric field –eE=ma.

$$a = \frac{-eE}{m}$$

It is clear from the above equation that the electrons are accelerated indefinitely because of growth of their velocity due to electric field i.e. its drift velocity v_d increases with time. However the electrons are not accelerated indefinitely because during their motion the electrons collide with impurities and lattice imperfections in the crystal. Here Drude assumed that the conduction electron acquires random motion after collision with impurities and lattice imperfections. In the collision process the electron loses the energy and after collision it again gains energy from the electric field. The velocity of the electrons after collision does not depend upon its velocity before collision. When the electron collides with the lattice imperfection it stops momentarily and moves in another direction with a new velocity. Thus electrons acquire random motion even in the presence of electric field. This problem can be solved by considering these collisions are similar to the collision process of an ideal gas in a container. The collision process introduces the concept of relaxation time, which influences the conductivity in the metals. The average time between successive collisions of electron with the lattice imperfection is called relaxation time and is denoted by τ.

The acceleration of the electron due to collision with impurities is given by $-v_d/\tau$ (negative sign is due to the acceleration is opposite to the direction of electric field). Now, the acceleration is equal to sum of the acceleration due to electric field and acceleration due to collision with impurities.

$$a = \frac{-eE}{m} - \frac{vd}{\tau}$$

After sometime the acceleration of the electrons due to the electric field and acceleration due to collision should compensate with each other but leads to steady state condition of the electron gas. As a result the acceleration of electron becomes zero

$$\frac{-eE}{m} - \frac{vd}{\tau} = 0$$

The drift velocity of the electron is then obtained by arranging the above equation.

$$v_d = \frac{-e\tau E}{m}$$

Thus the electrons in a conductor attain a constant drift velocity under the application of the electric field. The drift velocity is proportional to applied electric field and the proportionality constant is called the electron mobility μ.

(ii) Electron Mobility (μ) :

The electron mobility is defined as the drift velocity v_d per unit applied electric field E.

$$\mu = \frac{vd}{E}$$

Substituting the value of dirft velocity in the above equation we get

$$\mu = \frac{-e\tau}{m}$$

The above equation shows that mobility of an electron depends on the relaxation time and hence it depends on temperature.

10 Minutes

Verify

1. Draw energy band structure for Copper and Magnesium.
2. Write microscopic and macroscopic forms of Ohm's law
3. Define drift velocity and mobility of electron and write the expression of electrical conductivity in metals.

30 Minutes

ELECTRICAL RESISTIVITY OF METALS :

The resistivity ρ is defined by scattering events due to the imperfections and thermal vibrations. Total resistivity ρ_{tot} can be described by the Matthiessen's rule:

$\rho_{total} = \rho_{thermal} + \rho_{impurity} + \rho_{deformation}$, Where $\rho_{thermal}$ - from thermal vibrations, $\rho_{impurity}$ - from impurities, $\rho_{deformation}$ - from deformation-induced defects resistivity increases with temperature, with deformation, and with alloying.

Graphical explanation to electrical resistivity in metals:

APPLICATIONS OF ELECTRICAL CONDUCTING MATERIALS

One of the best materials for electrical conduction (low resistivity) is silver, but its use is restricted due to the high cost. Most widely used conductor is copper: inexpensive, abundant, high σ, but rather soft – cannot be used in applications where mechanical strength is important.

Metal	*Electrical Conductivity* $[(\Omega\text{-}m)^{-1}]$
Silver	6.8×10^7
Copper	6.0×10^7
Gold	4.3×10^7
Aluminum	3.8×10^7
Iron	1.0×10^7
Brass (70 Cu–30 Zn)	1.6×10^7
Platinum	0.94×10^7
Plain carbon steel	0.6×10^7

Table 3.1: Room temperature electrical conductivities for eight common metals and alloys

Solid solution alloying and cold working improve strength but decrease conductivity. If hardeningis preferred, Cu-Be alloy is used. When weight is important one uses aluminum, which is half as good as Cu and more resistant to corrosion. Heating elements require low (high R), and resistance to high

temperature oxidation: nickel chromium alloy.

10 Minutes

Verify

1) Discuss the origin of electrical resistance in metals.
2) Explain variation of electrical resistance of a metal with change of temperature?
3) Compare the influence of temperature, impurity concentration and deformation on electrical resistance of metals.

Session 12 : Semiconductors and conductivity

30 Minutes

Classification - conductivity (Board Teaching)

SEMI CONDUCTORS

INTRODUCTION (10 min)

The electrical conductivity of the semiconducting materials is not as high as that of the metals. Nevertheless they have some unique electrical characteristics that render them especially useful. The electrical properties of these materials are extremely sensitive to the presence of even minute concentrations of impurities.

Intrinsic Semiconductors (20 min):

Intrinsic semiconductors - electrical conductivity is defined by the electronic structure of pure material.

Extrinsic semiconductors - electrical conductivity is defined by impurity atoms.

Intrinsic semiconductors

Highly pure semiconductors with no impurities are called intrinsic semiconductors. In such a material there are no charge carriers at 0K. Since the valence band is filled and the conduction band is empty. At higher temperatures, the electrons reaching the conduction band due to thermal excitation leave equal number of holes in valence band. In intrinsic semiconductor, the number of free electrons is equal to the number of holes. The bond structure and band structures of intrinsic semiconductors are shown in below fig 3.15.

Examples: Si, Ge, GaP, GaAs, InSb, CdS, ZnTe

(a) (b)

Figure 3.15: (a) For a semiconductor, occupancy of electron states after an electron excitation from the valence band into the conduction band in which both a free electron and a hole are generated. (b) Electron bonding model of electrical conduction in intrinsic silicon after excitation.

Number of electrons in the conduction band increases exponentially with temperature.E_g is the band-gap width. In an electric field, electrons and holes move in opposite direction and participate in conduction.Since both electrons and holes are charge carriers in an intrinsic semiconductor, the conductivity is

$$\sigma = n|e|\mu_e + p|e|\mu_h$$

where p is the hole concentration and μ_h the hole mobility.

Electrons are more mobile than holes, $\mu_e > \mu_h$In an intrinsic semiconductor, a hole is produced by thepromotion of each electron to the conduction band. Therefore, **n = p**and (only for intrinsic semiconductors)

$$\sigma = n|e|(\mu_e + \mu_h) = p|e|(\mu_e + \mu_h)$$

n (and p) increase exponentially with temperature, whereas μ_e and μ_h decrease (about linearly) with temperature.The conductivity of intrinsic semiconductors is increasing with temperature (different from metals)

$$\sigma = n|e|(\mu_e + \mu_h)$$

Extrinsic semiconductors

The application of intrinsic semiconductors is restricted due to its low conductivity. In electronic devices, high conducting semiconductors are more essential. The concentration of either electrons or holes in a semiconductor should be increased depending upon the requirements in the electronic devices.

This can be carried out simply by adding impurities (one atom in 10^7 host atoms) to the intrinsic semiconductors. The process of adding impurity to the intrinsic semiconductors is called doping. The doped semiconductor is called as extrinsic semiconductor. The concentration of electrons and holes are not equal in an extrinsic semiconductor.

Usually the doping material is either penta-valent atoms (P, AS, Sb, Bi) or trivalent atoms (B, Al, Ga, In). The penta-valent atom is called donor atom because it donates one electron to the conduction band of pure semiconductor. The trivalent doping atom is called acceptor atom because it accepts one electron from semiconductor atom. The added impurity is called dopant.

In Extrinsic semiconductors, electrical conductivity is defined by impurity atoms.

Example: Si is considered to be extrinsic at room T if impurity concentration is one impurity per 10^{12} lattice sites (remember our estimation of the number of electrons promoted to the conduction band by thermal fluctuations at 300 K) unlike intrinsic semiconductors, an extrinsic semiconductor may have different concentrations of holes and electrons. It is called p-type if $p > n$ and n-type if $n > p$.

Thus there are two types of extrinsic semiconductors depending on the type of impurity added (10 min).

1. N-type extrinsic semiconductors
2. P-type extrinsic semiconductors

N-type extrinsic semiconductors:

Excess electron carriers are produced by substituting impurities that have more valence electron per atom than the semiconductor matrix.

Example: phosphorus (or As, Sb) with 5 valence electrons, is an electron donor in Si since only 4 electrons are used to bond to the Si lattice when it substitutes for a Si atom. Fifth outer electron of P atom is weakly bound in a donor state(~ 0.01 eV) and can be easily promoted to the conduction band.Impurities which produce extra conduction electrons are called donors,Elements in columns V and VI of the periodic table are donors for semiconductors in the IV column, Si and Ge.

The hole created in donor state is far from the valence band and is immobile. Conduction occurs mainly by the donated electrons thus n-type.

Figure 3.16: Extrinsic n-type semi conduction model (electron bonding). An impurity atom such as phosphorus, having five valence electrons, may substitute for a silicon atom.

(a) (b)

Figure 3.17: (a) Electron energy band scheme for a donor impurity level located within the band gap and just below the bottom of the conduction band. (b) Excitation from a donor state in which a free electron is generated in the conduction band.

P-type extrinsic semiconductors:

Excess holes are produced by substituting impurities that have fewer valence electrons per atom than the matrix. A bond with the neighbors is incomplete and can be viewed as a holeweakly bound to the impurity atom. Elements in columns III of the periodic table (B, Al, Ga) are donors for semiconductors in the IV column, Si and Ge. Impurities of this type are called acceptors.

(a) (b)

Figure 3.18: (a) Energy band scheme for an acceptor impurity level located within the band gap and just above the top of the valence band. (b) Excitation of an electron into the acceptor level leaving behind a hole in the valence band.

Figure 3.19: Extrinsic p-type semi conduction model (electron bonding). An impurity atom such as boron having three valence electrons, may substitute for a silicon atom.

The energy state that corresponds to the hole (acceptor state) is close to the top of the valence band. An electronmay easily jump from the valence band to complete the bondleaving a hole behind. Conduction occurs mainly by theholes (thus p-type). For extrinsic p-type semiconductors

$\sigma = p|e|\mu_p$

10 Minutes

Verify

1) Explain the conductivity and resistivity of different types of semiconductors.

2) Compare the temperature dependence of the conductivity for metals and intrinsic semiconductors. Briefly explain the difference in behavior.
3) Draw energy band stucture of n-type and p-type semiconductors.
4) Compare the temperature dependence of the conductivity for metals and intrinsic semiconductors. Briefly explain the difference in behavior.

30 Minutes

Factors effecting conductivity of semiconductors

1) Temperature effect on concentration of charge carrier in intrinsic and extrinsic semiconductors.
2) Effect of concentration of charge carriers on mobility of charge carriers.
3) Effect of temperature on mobility of charge carriers

(Please refer Callister's Materials science and engineering - An Introduction)

10 Minutes

Verify

1. State the reason for increase of electrical conductivity with increase of temeperature in intrinsic semiconductor.
2. State the reason for decrease of mobility with increase of concentration of charge carriers and temperature.
3. Explain the resons for no change in carrier concentration with increase of temperature in extrinsic region.

Session 13: Basic definitions in Dielectrics, relations and Polarization

30 Minutes

DIELECTRICS (Board Teaching)

All dielectric materials are electrical insulators. But all electric insulators need not be dielectrics. Ex: Vacuum is an insulator but it is not dielectric.The distinction between a dielectric material and an insulator lies in the application. The insulating materials are used to resist the flow of current through

1. *A short sketch of laser history*

1917: Einstein – stimulated absorption and emission of light

1954: Charles Townes and Schawlow – maser, prediction of the optical laser - Nobel Prize (1964)

1960: Maimann – first demonstration of a laser: Ruby laser

Rapid progress in the 1960s:

1961: first gas laser, first Nd laser

1962: first semiconductor laser

1963: CO_2 laser (IR)

2. *Introduction*

- A laser is a device that generates light by a process called **STIMULATED EMISSION**.
- The acronym LASER stands for Light Amplification by Stimulated Emission of Radiation

3. *Characteristic of laser*

Th The laser light exhibits some peculiar properties than compare with the convectional light. Those are

- Highly directionality
- Highly monochromatic
- Highly intense
- Highly coherence

Highly directionality

- The light ray coming ordinary light source travels in all directions, but laser light travels in single direction.
- For example the light emitted from torch light travels 1km distance it spreads around 1 km wide.
- But the laser light spreads a few centimetres distance even it travels lacks of kilometre distance.

- The directionality of laser beam is expressed in terms of divergence Ø

$$\phi = \frac{arc}{radius} = \frac{d_2 - d_1}{s_2 - s_1}$$

- Where d_2 and d_1 are the diameters of laser spots at distances of s_2 and s_1 respectively from laser source.
- For laser light divergence $\phi = 10^{-3} radians$.
- Since the divergence of light is very low, so we say that the laser light having highly directional.

Highly monochromatic

- In laser radiation, all the photons emitted between discrete energy levels will have same wavelength.
- As a result the radiation is monochromatic in nature.
- Due to the stimulated characteristic of laser light, the laser light is more monochromatic than that of a convectional light.
- laser radiation -the wavelength spread = 0.001 nm
- So it is clear that the laser radiation is highly monochromatic

Highly intense

- Laser light is highly intense than the convectional light.
- one mill watt He-Ne laser is highly intense than the sun intensity
- when two photons each of amplitude are in phase with other; the resultant amplitude of two photons is **2a** and the intensity is **$4a^2$**
- in laser much number of photons are in phase with each other, the amplitude of the resulting wave becomes na and hence the intensity of laser is proportional to **n^2a^2**
- So 1mW He-Ne laser is highly intense than the sun

Highly coherence

- Coherence is the property of the wave being in phase with itself and also with another wave over a period of time, and space or distance. There are two types of coherence
- Temporal coherence
- Spatial coherence.
- For laser radiation all the emitted photons are in phase, the resultant radiation obeys spatial and temporal coherence.

Temporal coherence (or longitudinal coherence):-

The predictable correlation of amplitude and phase at one point on the wave train w .r. t another point on the same wave train, then the wave is said to be temporal coherence.

spatially coherence (or transverse coherence).

The predictable correlation of amplitude and phase at one point on the wave train w. r .t another point on a second wave, then the waves are said to be spatially coherence (or transverse coherence).

4. *Stimulated absorption*

Let E_1 and E_2 **are** the energies and N_1 and N_2 are the number of atoms per unit volume of ground and excited states and ρ (υ) be the density of photon density.

Suppose, if a photon of energy $E_2 - E_1 = h\upsilon$ interacts with an atom present in the ground state, the atom gets excitation form ground state to excited state by absorbing the photon energy.

It is the *process of excitation of atom into excited state from ground state by absorbing the incident photon*.

Stimulated absorption rate depends upon the number of atoms available in the lowest energy state as well as the energy density photons.

Stimulated absorption rate $\propto N_1$

$\propto \rho$ (υ)

$\propto \rho(\upsilon)\, N_1$

$= B_{12}\, \rho(\upsilon)\, N_1$

Where B_{12} is known as Einstein coefficient of stimulated absorption

5. *Spontaneous emission*

- Spontaneous emission was postulated by Bohr.
- The excited atom does not stay in a long time in the excited state.
- The lifetime of excited atom in higher state E_2 is up to 10^{-8} seconds.
- After the life time of the excited atom, gets de-excited into ground by emitting a photon of energy $E_2 - E_1 = h\upsilon$.

It is the process of de-excitation of atom itself into ground state after its life time from excited state by emitting a photon

Spontaneous emission rate $\propto N_2$

$= A_{21} N_2$

Where A_{21} is known as Einstein coefficient of spontaneous emission

Characteristics of spontaneous emitted radiation

- The emitted radiation is poly-monochromatic
- The emitted radiation is Incoherent
- The emitted radiation is less intense
- The emitted radiation has less directionality
- Example: light from sodium or mercury lamp

6. *Stimulated emission*

Stimulated emission was postulated by Einstein.

Let, a photon of energy $E_2 - E_1 = h\upsilon$ interacts with the excited atom with in their life time; the atom gets de-excitation into ground state by emitting of additional photon.

It is the *process of de-excitation of atom into ground state from excited state by interacting with an additional photon within its life time by emitting of an additional photon.*

Stimulated emission rate depends upon the number of atoms available in the excited state as well as the energy density of photons.

Stimulated emission rate $\propto N_2$

$\propto \rho$

$\propto N_2 \rho$

$= B_{21} N_2 \rho$

Where B_{21} is known as Einstein coefficient of stimulated emission

Characteristics of stimulated emitted radiation

- The emitted radiation is monochromatic
- The emitted radiation is Coherent
- The emitted radiation is high intense
- The emitted radiation has high directionality
- Example: light from laser source

7. *Spontaneous and Stimulated emission*

Spontaneous emission	Stimulated emission
1. The spontaneous emission was postulated by Bohr	1. The stimulated emission was postulated by Einstein
2. Additional photons are not required in spontaneous emission	2. Additional photons are required in stimulated emission
3. One photon is emitted in spontaneous emission	3. Two photons are emitted in stimulated emission
4. The emitted radiation is poly-monochromatic	4. The emitted radiation is monochromatic
5. The emitted radiation is Incoherent	5. The emitted radiation is Coherent
6. The emitted radiation is less intense	6. The emitted radiation is high intense
7. The emitted radiation have less directionality	7. The emitted radiation have high directionality
8. Example: : light from sodium or mercury lamp	8. Example: light from laser source

9. *Population inversion*

Let us consider two level energy system of energies E_1 and E_2 as shown in figure. Let N_1 and N_2 be the populations of energy levels E_1 and E_2. The number of atoms present in an energy level is known as population of that energy level. At ordinary conditions, i.e., the population in the ground or lower state is always greater than the population in the excited or higher states. The stage of making, population of higher energy level is greater than the population of lower energy level is called population inversion.

According to Boltzmann's distribution the population of an energy level E_i at temperature T is given by

$$N_i = N_0 e^{\left(\frac{-E_i}{KT}\right)}$$

Where N_0 *is* the population of the lower level or ground state and k is is the Boltzmann's constant.

The number of atoms present in the excited state (N_2) is greater than the number of atoms present in the ground state (N_1) is called population inversion.

The process of raising the particles from ground state to excited state to achieve population inversion is called pumping. (Or the process of achieving of population inversion is called pumping)

To understand the concept of laser emission (stimulated emission) let us consider a three energy level system with energies E_1, E_2 and E_3 of populations, N_1, N_2 and N_3.At normal conditions, $E_1 < E_2 < E_3$ and $N_1 < N_2 < N_3$. In the ground state the life time of atom is more and the life time of atom in the excited state is 10^{-8}sec. But in the intermediate state the atom has more life time. So it is called metastable state.

At normal conditions $N_1 > N_2 > N_2$ **After population inversion is achieved** $N_2 > N_1$

When a suitable energy is supplied to the system, atoms get excited into E_3. After their lifetime the atoms are transit into E_2. Due to more lifetime of an atom in state E_2, the atoms stay for longer time than compare with the state E_3. Due to the accumulation of atoms instate E_2, the population inversion is established in between the E_1 and E_2 states.

10. Types of lasers

On the basis of active medium used in the laser systems, lasers are classified into several types

I. Solid lasers : Ruby laser, Nd;YAG laser, Nd;Glass
II. Liquid lasers : Europium Chelate laser, $SeOCl_2$
III. Gas lasers : CO_2, He-Ne, Argon-Ion Laser
IV. Dye lasers : Rhodamine 6G
V. Semiconductor lasers : InP, GaAs.
VI. Chemical lasers : HF, DF.

11. Construction and components of laser

Generally, every laser system consists of three components. They are

a. Energy source
b. Active medium
c. Optical cavity or resonator

Energy source

- To get laser emission, first we must have population inversion in the active medium.
- The energy source supplies the energy to the active medium.
- By absorbing that energy, the atoms or molecules or ions can be excited into higher levels.
- As a result we get population inversion in the active medium.

Active medium

Definition: - ***In which medium we are creating population inversion to get stimulated emission of radiation is called active medium.***

- After receiving the energy from the source, the atoms or molecules or ions get excites into higher energy levels.
- While de-excitation to lower energy level, the emitted photons starts stimulated emission which results laser emission.
- Depending upon the active medium the lasers or classified as solid state, liquid state, gaseous state and semiconductor lasers.

Optical cavity or resonator

- ***The active medium is enclosed between a fully reflective mirror and partially reflective mirror. These mirrors constitute the optical cavity or resonator.***
- The reflectors enhance the stimulated emission process by reflecting the photons into the active medium.
- As a result we get high-intensity monochromatic and coherent laser light through the partially reflecting portion of the mirror.

12. Excitation mechanisms

Excitation of atom can be done by number of ways. The most commonly used excitation methods are

- Optical pumping
- Electrical discharge pumping
- Chemical pumping
- Injection current pumping

Optical pumping

- Optical pumping is a process in which light is used to raise the atoms from a lower energy level to higher level to create population inversion.
- Optical pumping is used in solid laser.
- The solid materials have very broad absorption band, so sufficient amount of energy is absorbed from the emission band of flash lamp to create population inversion.
- Xenon flash tubes are used for optical pumping.
- Examples: - Ruby laser, Nd:YAG Laser (Neodymium: Yttrium Aluminum Garnet), Nd: Glass Laser

Electrical discharge pumping

- In electric discharge pumping, atoms are excited into excited sate by collisions with fast moving electrons in electric discharge tube.
- Electrical discharge pumping is used in gas lasers.
- Since gas lasers have very narrow absorption band, so optical pumping is not suitable for gas lasers.
- Examples:- He-Ne laser, CO_2 laser, argon-ion laser, etc

Chemical pumping

- In this method the chemical energy released during the chemical process, that energy will excite the atoms to higher level and create population inversion.
- Whenever hydrogen reacts with fluorine, it liberates lot of heat energy. By utilizing this heat energy the atoms excites into higher states and create population inversion.
- Examples:-HF and DF lasers.

Injection current pumping

- This pumping mechanism is used in semiconductor lasers.
- In semiconductor lasers, by passing high currents across the junction, the population inversion will create.
- In semiconductors lasers the population inversion always creates among majority and minority charge carriers.
- Examples:- InP and GaAs lasers

6. Ruby laser

Ruby laser is a three level solid state laser and was constructed by Mainmann in 1960. Ruby (Al_2O_3+Cr_2O_3) is a crystal of Aluminium oxide, in which 0.05% of Al^{+3} ions are replaced by the Cr^{+3} ions. The colour of the rod is pink. The active medium in the ruby rod is Cr^{+3} ions.

Construction

In ruby laser 4cm length and 5mm diameter rod is generally used. Both the ends of the rods are highly polished and made strictly parallel. The ends are silvered in such a way, one becomes partially reflected and the other end fully reflected. The ruby rod is surrounded by xenon flash tube, which provides the pumping light to excite the chromium ions in to upper energy levels.

Xenon flash tube emits thousands joules of energy in few milli seconds, but only a part of that energy is utilized by the chromium ions while the rest energy heats up the apparatus. A cooling arrangement is provided to keep the experimental set up at normal temperatures

Working

The energy level diagram of chromium ions is shown in figure.

The chromium ions get excitation into higher energy levels by absorbing of 5600A^0 of wave length radiation. The excited chromium ions stay in the level H for short interval of time (10^{-8} Sec). After their life time most of the chromium ions are de-excited from H to G and a few chromium ions are de-excited from H to M.

The transition between H and M is non-radioactive transition i.e. the chromium ions gives their energy to the lattice in the form of heat. In the Meta stable state the life time of chromium ions is 10^{-3} sec. The life time of chromium ions in the Meta stable state is 10^5 times greater than the life time of chromium ions in higher state.

Due to the continuous working of flash lamp, the chromium ions are excited to higher state H and returned to M level. After few milli seconds the level M is more populated than the level G and hence the desired population inversion is achieved. The state of population inversion is not a stable one. The process of spontaneous transition is very high. When the excited chromium ion passes spontaneously from H to M it emits one photon of wave length $6943A^0$. The photon reflects back and forth by the silver ends and until it stimulates an excited chromium ion in M state and it to emit fresh photon in phase with the earlier photon. The process is repeated again and again until the laser beam intensity is reached to a sufficient value. When the photon beam becomes sufficient intense, it emerges through the partially silvered end of the rod. The wave length $6943A^0$ is in the red region of the visible spectrum.

Draw backs of ruby laser

- The laser requires high pumping power
- The efficiency of ruby laser is very small
- It is a pulse laser

Uses o ruby laser

1. Ruby lasers are in optical photography
2. Ruby lasers can be used for measurement of plasma properties such as electron density and temperature.
3. Ruby lasers are used to remove the melanin of the skin.
4. Ruby laser can be used for recording of holograms.

14. Semiconductor diode laser

- Laser diode is a specially fabricated *p-n* junction device that emits coherent radiation.
- It is operated at forward biased condition.
- Direct band gap semiconductors are preferred in the fabrication of semiconductor laser diodes because they emit energy in terms of light when an electron and hole recombination takes place.
- Compound semi-conductors like GaAs and InP are examples for direct band gap semiconductors

Construction

- In this laser system, the active medium is a p-n junction diode made from crystalline gallium arsenide.
- The p-region and n-region in the diode are obtained by heavily doping with germanium and tellurium respectively in GaAs.
- The thickness of the p-n junction is very narrow so that the emitted radiation has large divergence and poor coherence.
- At the junction two sides are roughed to avoid laser emission and the remaining two faces one is partially polished and the other is fully polished.
- The laser emission takes place from the partially polished face.
- To provide bias two metal contacts are provided in the top and bottom of the diode as shown in figure.

Working

- The semiconductor laser device is always operated in forward bias condition.
- Electrons and the holes are the minority charge carriers in n-region and p-region semiconductors.
- When a huge current (10^4 Amp/mm^2) is passing through the p-n junction, p-region is positively biased, holes are injected into n-region from p-region and n-region is negatively biased electrons are injected into p-region from n-region as shown in figure.

- The continuous injection of charge carriers creates the population inversion of minority carriers in n and p sides' respectively.
- The electrons and holes recombine and release of light energy takes place in or near the junction as shown in figure.
- The emitted photons increase the rate of recombination of injected electrons from the n-region and holes in p-region by inducing more recombinations.

  From Planck's law $E_g = hv = h\frac{C}{\lambda}$

  $$\lambda = \frac{hC}{E_g} = \frac{6.63 \times 10^{-34} \times 3 \times 10^{8}}{1.4 \times 1.6 \times 10^{-19}} = 8874A^0$$

- In case of GaAs homo-junction which has an energy gap of 1.44eV gives a laser beam of wave length around 8874A^0.
- The wave length of emitted radiation depends up on the concentration of donor and acceptor atoms in GaAs.
- The efficiency of the laser emission is increases when we cool the GaAs diode.

16. Applications of lasers

Due to high intensity, high monocromacity and high directionality of lasers, they are widely used in various fields like

1. communication
2. computers
3. chemistry
4. photography
5. industry
6. medicine
7. military
8. scientific research

1. communication

In case of optical communication semiconductors laser diodes are used as optical sources and its band width is (10^{14}Hz) is very high compared to the radio and microwave communications.

- More channels can be sent simultaneously
- Signal cannot be tapped
- As the band width is large, more data can be sent.
- A laser is highly directional and less divergence, hence it has greater potential use in space crafts and submarines.

2. Computers

- In LAN (local area network), data can be transferred from memory storage of one computer to other computer using laser for short time.
- Lasers are used in CD-ROMS during recording and reading the data.

3. Chemistry

- Lasers are used in molecular structure identification
- Lasers are also used to accelerate some chemical reactions.
- Using lasers, new chemical compounds can be created by breaking bonds between atoms are molecules.

4. Photography

- Lasers are also used in the construction of holograms.
- Lasers can be used to get 3-D lens less photography.

5. Industry

- Lasers can be used to blast holes in diamonds and hard steel
- Lasers are also used as a source of intense heat
- Lasers are used to drill holes in ceramics.
- Lasers are used to cut glass and quartz.
- Lasers are used for heat treatment in the tooling and automotive industry.
- Lasers are used in electronic industry in trimming the components of ICS.
- High power lasers are used to weld or melt any material.
- Lasers are also used to cut teeth in saws and test the quality of fabric.

6. Medicine

- Lasers are used for cataract removal.
- Lasers are used for eye lens curvature corrections.
- Lasers are used in bloodless surgery.
- Lasers are used in cancer diagnosis and therapy.
- Lasers are used in destroying kidney stones and gallstones.
- Argon and carbon dioxide lasers are used in the treat men of liver and lungs.
- Lasers used in endoscopy to scan the inner parts of the stomach.
- Lasers used in the elimination of moles and tumours which are developing in the skin tissue.
- Lasers are used in plastic surgery.
- Lasers are used in the treatment of mouth diseases.

7. Military

- Lasers can be used as a war weapon.
- High energy lasers are used to destroy the enemy air-crofts and missiles.
- Lasers can be used in the detection and ranging likes RADAR.

8. **Scientific field**

- Lasers are used for isotope preparation.
- Lasers are employed to create plasma.
- Lasers are used in air pollution, to estimate the size of the dust particles.
- Lasers are used in the field of 3D-photography
- Lasers used in Recording and reconstruction of hologram.
- Lasers used to produce certain chemical reactions.
- Lasers are used in Raman spectroscopy to identify the structure of the molecule.
- Lasers are used in the Michelson- Morley experiment.

Body-centered cubic problems

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Problem #1: The edge length of the unit cell of Ta, is 330.6 pm; the unit cell is body-centered cubic. Tantalum has a density of 16.69 g/cm^3.

(a) calculate the mass of a tantalum atom.
(b) Calculate the atomic weight of tantalum in g/mol.

Solution:

1) Convert pm to cm:

330.6 pm x 1 cm/10^{10} pm = 330.6 x 10^{-10} cm = 3.306 x 10^{-8} cm

2) Calculate the volume of the unit cell:

(3.306 x 10^{-8} cm)^3 = 3.6133 x 10^{-23} cm^3

3) Calculate mass of the 2 tantalum atoms in the body-centered cubic unit cell:

16.69 g/cm^3 times 3.6133 x 10^{-23} cm^3 = 6.0307 x 10^{-22} g

4) The mass of one atom of Ta:

6.0307 x 10^{-22} g / 2 = 3.015 x 10^{-22} g

5) The atomic weight of Ta in g/mol:

3.015 x 10^{-22} g times 6.022 x 10^{23} mol^{-1} = 181.6 g/mol

---

Problem #2a: Chromium crystallizes in a body-centered cubic structure. The unit cell volume is 2.583 x 10^{-23} cm^3. Determine the atomic radius of Cr in pm.

Solution:

1) Determine the edge length of the unit cell:

2.583 x 10^{-23} cm^{3}3 = 2.956 x 10^{-8} cm

2) Examine the following diagram:

The triangle we will use runs differently than the triangle used in fcc calculations.
d is the edge of the unit cell, however d√2 is NOT an edge of the unit cell. It is a
diagonal of a face of the unit cell. 4r is a body

diagonal. Since it is a right triangle, the Pythagorean Theorem works just fine.

We wish to determine the value of 4r, from which we will obtain r, the radius of the Cr atom. Using the Pythagorean Theorem, we find:

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = (4r)^2$

$3(2.956 \times 10^{-8}\ cm)^2 = 16r^2$

$r = 1.28 \times 10^{-8}$ cm

3) The conversion from cm to pm is left to the student.

Problem #2b: Chromium crystallizes with a body-centered cubic unit cell. The radius of a chromium atom is 128 pm . Calculate the density of solid crystalline chromium in grams per cubic centimeter.

Solution:

1) Convert pm to cm:

$(125\ pm)\ (1\ cm / 10^{10}\ pm) = 1.25 \times 10^{-8}$ cm

2) Use the Pythagorean theorem to calculate the unit cell edge length:

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = (4r)^2$

$3d^2 = 16r^2$

$3d^2 = (16)\ (1.25 \times 10^{-8}\ cm)^2$

$d3 = (4)\ (1.25 \times 10^{-8}\ cm)$

$d = [(4)\ (1.25 \times 10^{-8}\ cm)] / 3$

$d = 2.8868 \times 10^{-8}$ cm

3) Calculate volume of the unit cell

$(2.8868 \times 10^{-8}\ cm)^3 = 2.4056 \times 10^{-23}\ cm^3$

4) Determine mass of two atoms in body-centered unit cell:

$51.996\ g/mol\ /\ 6.022 \times 10^{23}\ atoms/mol = 8.63434 \times 10^{-23}\ g/atom$

8.63434×10^{-23} g/atom times 2 = 1.726868×10^{-22} g

5) Determine the density:

$1.726868 \times 10^{-22}\ g\ /\ 2.4056 \times 10^{-23}\ cm^3 = 7.18\ g/cm^3$ (to three sig figs)

Book value is 7.15.

Problem #3: Barium has a radius of 224 pm and crystallizes in a body-centered cubic structure. What is the edge length of the unit cell? (This is the reverse of problem #4.)

Solution:

1) Calculate the value for 4r (refer to the above diagram):

radius for barium = 224 pm

4r = 896 pm

2) Apply the Pythagorean Theorem:

$d^2 + (d2)^2 = (896)^2$

$3d^2 = 802816$

$d^2 = 267605.3333...$

d = 517 pm

Problem #4: Metallic potassium has a body-centered cubic structure. If the edge length of unit cell is 533 pm, calculate the radius of potassium atom. (This is the reverse of problem #3.)

Solution:

1) Solve the Pythagorean Theorem for r (with d = the edge length):

$d^2 + (d2)^2 = (4r)^2$

$d^2 + 2d^2 = 16r^2$

$3d^2 = 16r^2$

$r^2 = 3d^2 / 16$

r = (d3) / 4

2) Solve the problem:

r = (5333) / 4

r = 231 pm

Problem #5: Sodium has a density of 0.971 g/cm^3 and crystallizes with a body-centered cubic unit cell. (a) What is the radius of a sodium atom? (b) What is the edge length of the cell? Give answers in picometers.

Solution:

1) Determine mass of two atoms in a bcc cell:

22.99 g/mol divided by 6.022 x 10^{23} mol^{-1} = 3.81767 x 10^{-23} g (this is the average mass of one atom of Na)

3.81767 x 10^{-23} g times 2 = 7.63534 x 10^{-23} g

2) Determine the volume of the unit cell:

7.63534 x 10^{-23} g divided by 0.971 g/cm^3 = 7.863378 x 10^{-23} cm^3

3) Determine the edge length, which is the answer to (b):

7.863378 x 10^{-23} cm^{3}3 = 4.2842 x 10^{-8} cm

4) Use the Pythagorean Theorem (refer to above diagram):

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = 16r^2$

$r^2 = 3(4.2842 \times 10^{-8})^2 / 16$

$r = 1.855 \times 10^{-8}$ cm

5) The radius of the sodium atom is 185.5 pm. The edge length is 428.4 pm. The manner of these conversions are left to the reader.

Problem #6: At a certain temperature and pressure an element has a simple body-centred cubic unit cell. The corresponding density is 4.253 g/cm^3 and the atomic radius is 1.780 Å. Calculate the atomic mass (in amu) for this element.

Solution:

1) Convert 1.780 Å to cm:

1.780 Å = 1.780 x 10^{-8} cm

2) Use the Pythagorean Theorem to calculate d, the edge length of the unit cell:

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = 16r^2$

$d^2 = (16/3)\ (1.780 \times 10^{-8}\ \text{cm})^2$

$d = 4.11 \times 10^{-8}$ cm

3) Calcuate the volume of the unit cell:

$(4.11 \times 10^{-8}\ cm)^3 = 6.95 \times 10^{-23}\ cm^3$

4) Calcuate the mass inside the unit cell:

$6.95 \times 10^{-23}\ cm^3$ times $4.253\ g/cm^3 = 2.95 \times 10^{-22}\ g$

5) Use a ratio and proportion to calculate the atomic mass:

2.95×10^{-22} g is to two atoms as 'x' is to $6.022 \times 10^{23}\ mol^{-1}$

x = 88.95 g/mol (or 88.95 amu)

Problem #7: Mo crystallizes in a body-centered cubic arrangement. Calculate the radius of one atom, given the density of Mo is 10.28 g /cm^3.

Solution:

1) Determine mass of two atoms in a bcc cell:

95.96 g/mol divided by $6.022 \times 10^{23}\ mol^{-1} = 1.59349 \times 10^{-22}$ g (this is the average mass of one atom of Mo)

1.59349×10^{-22} g times 2 = 3.18698×10^{-22} g

2) Determine the volume of the unit cell:

3.18698×10^{-22} g divided by $10.28\ g/cm^3 = 3.100175 \times 10^{-23}\ cm^3$

3) Determine the edge length:

$3.100175 \times 10^{-23}\ cm^3 3 = 3.14144 \times 10^{-8}$ cm

4) Use the Pythagorean Theorem (refer to above diagram):

$d^2 + (d2)^2 = (4r)^2$

$3d^2 = 16r^2$

$r^2 = 3(3.14144 \times 10^{-8})^2 / 16$

$r = 1.3603 \times 10^{-8}$ cm (or 136.0 pm, to four sig figs)

Problem #8: Sodium crystallizes in body-centered cubic system, and the edge of the unit cell is 430. pm. Calculate the dimensions of a cube that would contain one mole of Na.

Solution:

A cube that is bcc has two atoms per unit cell.

6.022×10^{23} atoms divided by 2 atoms/cell = 3.011×10^{23} cells required.

430. pm = 4.30×10^{-8} cm <--- I'm going to give the answer in cm^3 rather than pm^3

$(4.30 \times 10^{-8}\ cm)^3 = 7.95 \times 10^{-23}\ cm^3$ <--- vol. of unit cell in cm^3

$(3.011 \times 10^{23}$ cell) $(7.95 \times 10^{-23}\ cm^3/cell) = 23.9\ cm^3$

$23.9\ cm^3$ would be a cube 2.88 cm on a side (2.88 being the cube root of 23.9)

Problem #9: Vanadium crystallizes with a body-centered unit cell. The radius of a vanadium atom is 131 pm. Calculate the density of vanadium in g/cm^3.

Solution:

1) We are going to use the Pythagorean Theorem to determine the edge length of the unit cell. That edge length will give us the volume.

131 pm times (1 cm / 10^{10} pm) = 131×10^{-10} cm = 1.31×10^{-8} cm

The right triangle for Pythagorean Theorem is here. The image is in problem #2.

$3d^2 = (4 * 1.31 \times 10^{-8}\ cm)^2$

$d^2 = (4 * 1.31 \times 10^{-8}\ cm)^2 / 3$

$d = 3.0253 \times 10^{-8}$ cm <--- this is the edge length

Cube the edge length to give the volume:

$2.7689 \times 10^{-23}\ cm^3$

2) We will use the average mass of one V atom and the two atoms in bcc to determine the mass of V inside the unit cell.

50.9415 g/mol divided by $6.022 \times 10^{23}\ mol^{-1} = 8.459 \times 10^{-23}$ g <--- average mass of one atom

8.459×10^{-23} g times 2 = 1.6918×10^{-22} g <--- mass of V in unit cell

3) Step 2 divided by step 1 gives the density.

$1.6918 \times 10^{-22}\ g / 2.7689 \times 10^{-23}\ cm^3 = 6.11\ g/cm^3$

Problem #10: Titanium metal has a body-centered cubic unit cell. The density of titanium is $4.50\ g/cm^3$. Calculate the edge length of the unit cell and a value for the atomic radius of titanium. (Hint: In a body-centered arrangement of spheres, the spheres touch across the body diagonal.)

Solution:

1) We need to determine the volume of one unit cell. I'll approach this in a dimensional analysis sorta way:

(volume/g) (g/mole) (mole/atoms) (atoms/cell) = (volume/cell)

See how all the units cancel except for volume and cell. Once we have the volume of the cell, we can determine the edge lenth by taking the cube root of the volume.

I'll build it one calculation at a time.

2) (volume/g)

$1.00\ cm^3/4.50\ g$

3) (volume/g) (g/mole) <--- molar mass of Ti

$(1.00\ cm^3/4.50\ g)\ (47.867\ g/mol)$

4) (volume/g) (g/mole) (mole/atoms) <--- Avogadro's Number

$(1.00\ cm^3/4.50\ g)\ (47.867\ g/mol)\ (1.00\ mol/6.022 \times 10^{23}\ atoms)$

5) (volume/g) (g/mole) (mole/atoms) (atoms/cell)

$(1.00\ cm^3/4.50\ g)\ (47.867\ g/mol)\ (1.00\ mol/6.022 \times 10^{23}\ atoms)\ (2\ atoms/cell)$ <--- because of body-centered cubic

6) Do the calculation for the volume of the unit cell. The answer is:

$3.53275 \times 10^{-23}\ cm^3$

7) The edge length is simply the cube root of the cell volume. The answer is:

3.28×10^{-8} cm (to three sig figs)

Comment: often the edge length is asked for in pm. The student is left to determine the conversion from cm to pm. The answer is 328 pm.

8) For the atomic radius, I will add some guard digits to the edge length (symbolized by 'd' in the Pythagorean theorem calculation I will use. By the way, remember that hint from the problem text? That's the thing that allows me to write 4r.

$d^2 + (d2)^2 = (4r)^2$

$(4r)^2 = 3d^2$

$16r^2 = 3d^2$

$r^2 = 3d^2 / 16$

$r = d3 / 4$

$r = [(3.28124 \times 10^{-8}\ cm)\ (3)] / 4$

$r = 1.42 \times 10^{-8}\ cm = 142\ pm$

Bonus Problem: In modeling solid-state structures, atoms and ions are most often modeled as spheres. A structure built using spheres will have some empty space in it. A measure of the empty (also called void) space in a particular structure is the packing efficiency, defined as the volume occupied by the spheres divided by the total volume of the structure.

Given that a solid crystallizes in a body-centered cubic structure that is 3.05 Å on each side, please answer the following questions.

Solution:

a. How many atoms are there in each unit cell?

2

b. What is the volume of one unit cell in $Å^3$?

$(3.05\ Å)^3 = 28.372625\ Å^3$

c. Assuming that the atoms are spheres and the radius of each sphere is 1.32 Å, what is the volume of one atom in $Å^3$?

$(4/3)\ (3.141592654)\ (1.32)^3 = 9.63343408\ Å^3$

I used the key for π on my calculator, so there were some internal digits in addition to that last 4 (which is actually rounded up from the internal digits).

d. Therefore, what volume of atoms are in one unit cell?

($9.63343408\ Å^3$ times 2) = $19.26816686\ Å^3$

e. Based on your results from parts b and d, what is the packing efficiency of the solid expressed as a percentage?

$19.26816686\ Å^3 / 28.372625\ Å^3 = 0.679$

67.9%

Go to a list of only the problems

Go to the face-centered cubic problems

Go to the general unit cell problems

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Face-centered cubic problems

Go to a list of only the problems

Go to some body-centered cubic problems

Go to some general unit cell problems

Return to the Liquids & Solids menu

Problem #1: Palladium crystallizes in a face-centered cubic unit cell. Its density is 12.023 g/cm^3. Calculate the atomic radius of palladium.

Solution:

1) Calculate the average mass of one atom of Pd:

$106.42 \text{ g mol}^{-1} \div 6.022 \times 10^{23} \text{ atoms mol}^{-1} = 1.767187 \times 10^{-22} \text{ g/atom}$

2) Calculate the mass of the 4 palladium atoms in the face-centered cubic unit cell:

1.767187×10^{-22} g/atom times 4 atoms/unit cell = 7.068748×10^{-22} g/unit cell

3) Use density to get the volume of the unit cell:

$7.068748 \times 10^{-22} \text{ g} \div 12.023 \text{ g/cm}^3 = 5.8793545 \times 10^{-23} \text{ cm}^3$

4) Determine the edge length of the unit cell:

$5.8793545 \times 10^{-23} \text{ cm}^3 3 = 3.88845 \times 10^{-8} \text{ cm}$

5) Determine the atomic radius:

Remember that a face-centered unit cell has an atom in the middle of each face of the cube. The square represents one face of a face-centered cube:

Here is the same view, with 'd' representing the side of the cube and '4r' representing the 4 atomic radii across the face diagonal.

Using the Pythagorean Theorem, we find:

$d^2 + d^2 = (4r)^2$

$2d^2 = 16r^2$

$r^2 = d^2 \div 8$

$r = d \div \sqrt{8}$ <--- often left like this

$r = d \div 2(\sqrt{2})$ <--- an alternate formulation

$r = 1.3748 \times 10^{-8}$ cm

You may wish to convert the cm value to picometers, the most common measurement used in reporting atomic radii. Try it before looking at the solution to the next problem.

The above discusses how to determine r in terms of d in a face-centered unit cell. You may be asked to do the opposite, that is, to determine d in terms of r for a fcc cell. I'll repeat:

$r = d \div \sqrt{8}$

followed by a simple rearrangement:

$d = r\sqrt{8}$

Problem #2: Nickel crystallizes in a face-centered cubic lattice. If the density of the metal is 8.908 g/cm^3, what is the unit cell edge length in pm?

Solution:

This problem is like the one above, it just stops short of determining the atomic radius.

1) Calculate the average mass of one atom of Ni:

$58.6934 \text{ g mol}^{-1} \div 6.022 \times 10^{23} \text{ atoms mol}^{-1} = 9.746496 \times 10^{-23}$ g/atom

2) Calculate the mass of the 4 nickel atoms in the face-centered cubic unit cell:

9.746496×10^{-23} g/atom times 4 atoms/unit cell = 3.898598×10^{-22} g/unit cell

3) Use density to get the volume of the unit cell:

3.898598×10^{-22} g ÷ 8.908 g/cm^3 = 4.376514×10^{-23} cm^3

4) Determine the edge length of the unit cell:

4.376514×10^{-23} cm^{3}3 = 3.524×10^{-8} cm

5) Convert cm to pm:

cm = 10^{-2} m; pm = 10^{-12} m.

Consequently, there are 10^{10} pm/cm

(3.524×10^{-8} cm) (10^{10} pm/cm) = 352.4 pm

Problem #3: Nickel has a face-centered cubic structure with an edge length of 352.4 picometers. What is the density?

This problem is the exact reverse of problem #2. (See problem 5a below for an example set of calculations.)

Solution:

1) Convert pm to cm
2) Calculate the volume of the unit cell
3) Calculate the average mass of one atom of Ni
4) Calculate the mass of the 4 nickel atoms in the face-centered cubic unit cell
5) Calculate the density (value from step 4 divided by value from step 2)

Problem #4: Calcium has a cubic closest packed structure as a solid. Assuming that calcium has an atomic radius of 197 pm, calculate the density of solid calcium.

Solution:

1) Convert pm to cm:

197 pm x (1 cm/10^{10} pm) = 1.97×10^{-8} cm

2) Determine the edge length of the unit cell:

Use the Pythagorean Theorem (see problem #1 for a discussion):

r = d ÷ 2(√2) <--- one of two alternate formulations

1.97×10^{-8} cm = d ÷ 2(√2)

d = 5.572×10^{-8} cm

3) Determine the volume of the unit cell:

(5.572×10^{-8} cm)^3 = 1.730×10^{-22} cm^3

4) Determine mass of 4 atoms of Ca in a unit cell (cubic closest packed is the same as face-centered cubic):

40.08 g/mol divided by 6.022×10^{23} atoms/mol = 6.6556×10^{-23} g/atom

6.6556×10^{-23} g/atom times 4 atoms = 2.66224×10^{-22} g

5) Determine density:

2.66224×10^{-22} g divided by 1.730×10^{-22} cm^3 = 1.54 g/cm^3

Problem #5: Krypton crystallizes with a face-centered cubic unit cell of edge 559 pm.

a) What is the density of solid krypton?
b) What is the atomic radius of krypton?
c) What is the volume of one krypton atom?
d) What percentage of the unit cell is empty space if each atom is treated as a hard sphere?

Solution to a:

1) Convert pm to cm:

559 pm x (1 cm/10^{10} pm) = 559×10^{-10} cm = 5.59×10^{-8} cm

2) Calculate the volume of the unit cell:

$(5.59 \times 10^{-8}\ cm)^3 = 1.7468 \times 10^{-22}\ cm^3$

3) Calculate the average mass of one atom of Kr:

83.798 g mol^{-1} divided by 6.022×10^{23} atoms mol^{-1} = 1.39153×10^{-22} g

4) Calculate the mass of the 4 krypton atoms in the face-centered cubic unit cell:

1.39153×10^{-22} g times 4 = 5.566×10^{-22} g

5) Calculate the density (value from step 4 divided by value from step 2):

5.566×10^{-22} g / 1.7468×10^{-22} cm^3 = 3.19 g/cm^3

Solution to b:

Use the Pythagorean Theorem (see problem #1 for a discussion):

r = d ÷ √8 <--- one of two alternate formulations

$r = 5.59 \times 10^{-8}$ cm ÷ √8

$r = 1.98 \times 10^{-8}$ cm

Solution to c:

$V = (4/3)\ \pi\ r^3$

$V = (4/3)\ (3.14159)\ (1.98 \times 10^{-8}\ cm)^3$

$V = 3.23 \times 10^{-23}\ cm^3$

Solution to d:

1) Calculate the volume of the 4 atoms in the unit cell:

$3.23 \times 10^{-23}\ cm^3$ times 4 = $1.29 \times 10^{-22}\ cm^3$

2) Calculate volume of cell not filled with Kr:

1.7468×10^{-22} cm^3 minus 1.29×10^{-22} cm^3 = 4.568×10^{-23} cm^3

3) Calculate % empty space:

4.568×10^{-23} cm^3 divided by 1.7468×10^{-22} cm^3 = 0.2615

26%

Problem #6: You are given a small bar of an unknown metal. You find the density of the metal to be 11.5 g/cm^3. An X-ray diffraction experiment measures the edge of the face-centered cubic unit cell as 4.06×10^{-10} m. Find the gram-atomic weight of this metal and tentatively identify it.

Solution:

1) Convert meters to cm:

4.06×10^{-10} m = 4.06×10^{-8} cm

2) Determine the volume of the unit cube:

$(4.06 \times 10^{-8}\text{ cm})^3 = 6.69234 \times 10^{-23}$ cm^3

3) Determine the mass of the metal in the unit cube:

11.5 g/cm^3 times 6.69234×10^{-23} cm^3 = 7.696193×10^{-22} g

4) Determine atomic weight (based on 4 atoms per unit cell):

7.696193×10^{-22} g is to 4 atoms as x grams is to 6.022×10^{23} atoms

x = 116 g/mol (to three sig figs)

This weight is close to that of indium.

Problem #7: A metal crystallizes in a face-centered cubic lattice. The radius of the atom is 0.197 nm. The density of the element is 1.54 g/cm^3. What is this metal?

Solution:

1) Convert nm to cm:

0.197 nm x (1 cm/10^7 nm) = 1.97×10^{-8} cm

2) Determine the edge length of the unit cell:

Use the Pythagorean Theorem (see problem #1 for a discussion):

$r = d \div 2(\sqrt{2})$ <--- one of two alternate formulations

1.97×10^{-8} cm = $d \div 2(\sqrt{2})$

d = 5.572×10^{-8} cm

3) Determine the volume of the unit cell:

$(5.572 \times 10^{-8}\ cm)^3 = 1.72995 \times 10^{-22}\ cm^3$

4) Determine grams of metal in unit cell:

$1.72995 \times 10^{-22}\ cm^3$ times $1.54\ g/cm^3 = 2.6641 \times 10^{-22}\ g$

5) Determine atomic weight (based on 4 atoms per unit cell):

2.6641×10^{-22} g is to 4 atoms as x grams is to 6.022×10^{23} atoms

x = 40.11 g/mol

The metal is calcium.

Problem #8: The density of an unknown metal is $2.64\ g/cm^3$ and its atomic radius is 0.215 nm. It has a face-centered cubic lattice. Determine its atomic weight.

Solution:

1) Convert nm to cm:

$0.215\ nm \times (1\ cm/10^7\ nm) = 2.15 \times 10^{-8}\ cm$

2) Determine the edge length of the unit cell:

Use the Pythagorean Theorem (see problem #1 for a discussion):

$r = d \div \sqrt{8}$ <--- one of two alternate formulations

$2.15 \times 10^{-8}\ cm = d \div \sqrt{8}$

$d = 6.08112 \times 10^{-8}\ cm$

3) Determine the volume of the unit cell:

$(6.08112 \times 10^{-8}\ cm)^3 = 2.2488 \times 10^{-22}\ cm^3$

4) Determine grams of metal in unit cell:

$2.2488 \times 10^{-22}\ cm^3$ times $2.64\ g/cm^3 = 5.9368 \times 10^{-22}\ g$

5) Determine atomic weight (based on 4 atoms per unit cell):

5.9368×10^{-22} g is to 4 atoms as x grams is to 6.022×10^{23} atoms

x = 89.4 g/mol

Problem #9: Metallic silver crystallizes in a face-centered cubic lattice with L as the length of one edge of the unit cube. What is the center-to-center distance between nearest silver atoms?

A) L / 2
B) $2^{½}$ L
C) 2L
D) L / $2^{½}$
E) None of the above answers are valid.

Solution:

Call center-to-center distance = d. There are two of them on the face diagonal.

Therefore, by the Pythagorean Theorem:

$L^2 + L^2 = (2d)^2$

$2L^2 = 4d^2$

$(L^2) / 2 = d^2$

$L / 2^{½} = d$

Answer choice D.

Problem #10: Iridium has a face-centered cubic unit cell with an edge length of 383.3 pm. The density of iridium is 22.61 g/cm^3. Use these data to calculate a value for Avogadro's Number.

Solution:

1) Use the edge length to get the volume of the unit cell:

383.3 pm = 3.833×10^{-8} cm

$(3.833 \times 10^{-8}\text{ cm})^3 = 5.6314 \times 10^{-23}\text{ cm}^3$

2) Use the density to get the mass of Ir in the unit cell:

22.61 g/cm^3 times 5.6314×10^{-23} cm^3 = 1.27326×10^{-21} g

3) Use the atomic weight of Ir to determine how many moles of Ir are in the unit cell:

1.27326×10^{-21} g divided by 192.217 g/mol = 6.624075×10^{-24} mol

4) Use 4 atoms per face-centered unit cell to set up the following ratio and proportion:

4 atoms is to 6.624075×10^{-24} mol as x is to 1.000 mol

x = 6.038×10^{23} atoms

For a different take on the solution to this problem, go here and take a look at the answer by Dr W.

Problem #11: Platinum has a density of 21.45 g/cm^3 and a unit cell side length 'd' of 3.93 Ångstroms. What is the atomic radius of platinum? (1 Å = 10^{-8} cm.)

Solution:

1) We need to determine if the unit cell is fcc or bcc.

Volume of unit cell:

$(3.93 \times 10^{-8}\text{ cm})^3 = 6.0698 \times 10^{-23}\text{ cm}^3$

Determine the mass of Pt in the unit cell:

21.45 g/cm^3 times 6.0698 x 10^{-23} cm^3 = 1.302 x 10^{-21} g

How many atoms is that?

(1.302 x 10^{-21} g / 195.078 g/mol) * 6.022 x 10^{23} mol^{-1} = 4

The unit cell for Pt is fcc.

2) Use the Pythogrean Theorem to calculate the length of the hypotenuse which we know to be four times the radii of one Pt atom (see Problem #1 for a discussion).

We know this:

$d^2 + d^2 = (4r)^2$ <--- where d is the edge length and r is the radius of the atom.

Therefore:

r = d ÷ 2(√2) <--- one of two alternate formulations

r = (3.93 x 10^{-8} cm) ÷ 2(√2)

r = 1.39 x 10^{-8} cm

3) Note that picometers is the preferred unit for atomic radii (with Ångstroms being the preferred unit of older vintage (for example, when the ChemTeam was in school).

1.39 x 10^{-8} cm equals:

139 pm
1.39 Å

Problem #12: The unit cell of platinum has a length of 392.0 pm along each side. Use this length (and the fact that Pt has a face-centered unit cell) to calculate the density of platinum metal in kg/m^3 (Hint: you will need the atomic mass of platinum and Avogadro's number).

Solution:

1) Calculate the volume of the unit cell in meters cubed:

392.0 pm times (1 m / 10^{12} pm) = 392.0 x 10^{-12} m = 3.920 x 10^{-10} m

(3.920 x 10^{-10} m)^3 = 6.0236288 x 10^{-29} m^3

2) Calculate the mass of Pt in the unit cell in kg:

195.078 g/mol divided by 6.022 x 10^{23} mol^{-1} = 3.239422 x 10^{-22} g

3.239422 x 10^{-22} g times 4 = 1.2957688 x 10^{-21} g

1.2957688 x 10^{-21} g times (1 kg / 1000 g) = 1.2957688 x 10^{-24} kg

3) Calculate the density:

1.2957688 x 10^{-24} kg / 6.0236288 x 10^{-29} m^3 = 21511 kg / m^3

The book value is 21450 kg / m^3.

Note the use of the SI-approved unit for density as opposed to the more commonly-used unit of g/cm^3.

Problem #13: A metal crystallizes in a face-centered cubic structure and has a density of 11.9 g cm^{-3}. If the radius of the metal atom is 138 pm, what is the most probable identity of the metal.

Solution:

1) Determine the atom radius in cm:

138 pm times (100 cm / 10^{12} pm) = 138 x 10^{-10} cm = 1.38 x 10^{-8} cm

2) Determine the edge length of the unit cell:

Use the Pythagorean Theorem (see problem #1 for a discussion):

r = d ÷ √8 <--- one of two alternate formulations

1.38 x 10^{-8} cm = d ÷ √8

d = 3.90323 x 10^{-8} cm

2) Determine the volume of the unit cell:

(3.90323 x 10^{-8} cm)^3 = 5.94665 x 10^{-23} cm^3

3) Determine the mass of the metal inside the unit cell:

11.9 g cm^{-3} times 5.94665 x 10^{-23} cm^3 = 7.0765 x 10^{-22} g

3) The above mass is that of 4 atoms (based on our knowledge that the unit cell is fcc). Scale the mass to that of Avogadro Number of atoms:

7.0765 x 10^{-22} g is to 4 atoms as x is to 6.022 x 10^{23} atoms/mole

x = 106.5 g/mol

The metal is palladium.

Problem #14: Nickel oxide (NiO) crystallizes in the NaCl type of crystal structure. The length of the unit cell of NiO is 4.20 Å. Calculate the density of NiO.

Solution:

1) A brief discussion . . .

. . . of the NaCl structure is found here. Ignore the question and the last half of the answer.

The key point is that in the NaCl unit cell, there are 4 Na^+ and 4 Cl^-. You can think of it as a face-centered unit cell of chloride ions has been interpenetrated with a face-centered unit cell of sodium ions.

Following the above, a unit cell of NiO will contain 4 Ni^{2+} and 4 O^{2-}

2) Convert Å to cm:

1 Å = 10^{-8} cm (Ångströn is an old unit but still used from time to time)

4.20 Å = 4.20×10^{-8} cm

3) The volume of one NiO unit cell is this:

$(4.20 \times 10^{-8}\ \text{cm})^3 = 7.4088 \times 10^{-23}\ \text{cm}^3$

4) The weight of four NiO in the unit cell:

$(74.692\ \text{g/mol} / 6.022 \times 10^{23}\ \text{mol}^{-1}) \times 4 = 4.96128 \times 10^{-22}$ g

5) Determine the density:

$4.96128 \times 10^{-22}\ \text{g} / 7.4088 \times 10^{-23}\ \text{cm}^3 = 6.70\ \text{g/cm}^3$

This compares to the book value of 6.67 g/cm^3

Problem #15: NiO adopts the face-centered-cubic arrangement. Given that the density of NiO is 6.67 g/cm^3, calculate the length of the edge of its unit cell (in pm).

Solution:

1) Calculate the average mass of one NiO formula unit:

74.692 g/mol divided by $6.022 \times 10^{23}\ \text{mol}^{-1} = 1.24032 \times 10^{-22}$ g

2) NiO has the NaCl structure, so 4 Ni and 4 O per unit cell. Determine the total mass of NiO in one unit cell:

$1.24032 \times 10^{-22}\ \text{g} \times 4 = 4.96128 \times 10^{-22}$ g

3) Determine the volume of the unit cell:

4.96128×10^{-22} g divided by 6.67 g/cm^3 = $7.4382 \times 10^{-23}\ \text{cm}^3$

4) Determine the edge length:

$7.4382 \times 10^{-23}\ \text{cm}^3 3 = 4.2055 \times 10^{-8}$ cm

5) Convert from cm to pm:

4.2055×10^{-8} cm times (10^{10} pm / 1 cm) = 420.55 pm

A value of 420. pm seems reasonable as a final answer.

Go to a list of only the problems

Go to some body-centered cubic problems

Go to some general unit cell problems

Return to the Liquids & Solids menu

If the atomic radius of lead is 0.175 nm, calculate the volume of its unit cell in cubic meters

4.1 For this problem, we are asked to calculate the volume of a unit cell of lead. Lead has an FCC crystal structure (Table 4.1). The FCC unit cell volume may be computed from Equation 4.4 as

$$V_C = 16R^3\sqrt{2} = (16)(0.175 \times 10^{-9}\ \text{m})^3(\sqrt{2}) = 1.213 \times 10^{-28}\ \text{m}^3$$

Molybdenum has a BCC crystal structure, an atomic radius of 0.1363 nm, and an atomic weight of 95.94 g/mol. Compute its density.

4.6 This problem calls for a computation of the density of molybdenum. According to Equation 4.5

$$\rho = \frac{nA_{\text{Mo}}}{V_C N_{\text{A}}}$$

For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 \qquad \rho = \frac{nA_{\text{Mo}}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_{\text{A}}}$$

Thus,

$$= \frac{(2\ \text{atoms/unit cell})(95.94\ \text{g/mol})}{\left[(4)(0.1363 \times 10^{-7}\ \text{cm})^3/\sqrt{3}\right]^3 /(\text{unit cell})(6.023 \times 10^{23}\ \text{atoms/mol})}$$

$$= 10.21\ \text{g/cm}^3$$

Calculate the radius of a palladium atom, given that Pd has an FCC crystal structure, a density of 12.0 g/cm^3, and an atomic weight of 106.4 g/mol.

4.7 We are asked to determine the radius of a palladium atom, given that Pd has an FCC crystal structure. For FCC, n = 4 atoms/unit cell, and $V_C = 16R^3\sqrt{2}$ (Equation 4.4). Now,

$$\rho = \frac{nA_{\text{Pd}}}{V_C N_{\text{A}}} = \frac{nA_{\text{Pd}}}{(16R^3\sqrt{2})N_{\text{A}}}$$

And solving for R from the above expression yields

$$R = \left(\frac{nA_{\text{Pd}}}{16\rho N_{\text{A}}\sqrt{2}}\right)^{1/3} = \left[\frac{(4\ \text{atoms/unit cell})(106.4\ \text{g/mol})}{(16)(12.0\ \text{g/cm}^3)(6.023 \times 10^{23}\ \text{atoms/mol})(\sqrt{2})}\right]^{1/3} = 1.38 \times 10^{-8}\ \text{cm} = 0.138\ \text{nm}$$

Calculate the radius of a tantalum atom, given that Ta has a BCC crystal structure, a density of 16.6 g/cm^3, and an atomic weight of 180.9 g/mol.

4.8 This problem asks for us to calculate the radius of a tantalum atom. For BCC, n = 2 atoms/unit cell, and

$$V_C = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

$$\rho = \frac{nA_{Ta}}{V_C N_A} = \frac{nA_{Ta}}{\left(\frac{64R^3}{3\sqrt{3}}\right)N_A}$$

$$R = \left(\frac{3\sqrt{3}nA_{Ta}}{64\rho N_A}\right)^{1/3} = \left[\frac{(3\sqrt{3})\,(2\text{ atoms/unit cell})\,(180.9\text{ g/mol})}{(64)\,(16.6\text{ g/cm}^3)(6.023\times10^{23}\text{ atoms/mol})}\right]^{1/3} = 1.43\times10^{-8}\text{ cm} = 0.143\text{ nm}$$

Some hypothetical metal has the simple cubic crystal structure shown in Figure. If its atomic weight is 74.5 g/mol and the atomic radius is 0.145 nm, compute its density.

4.9 For the simple cubic crystal structure, the value of n in Equation 4.5 is unity since there is only a single atom associated with each unit cell. Furthermore, for the unit cell edge length, $a = 2R$ (Figure 4.38). Therefore, employment of Equation 4.5 yields

$$\rho = \frac{nA}{V_C N_A} = \frac{nA}{(2R)^3 N_A} = \frac{(1\text{ atom/unit cell})(74.5\text{ g/mol})}{\left\{\left[(2)(1.45\times10^{-8}\text{ cm})\right]^3/(\text{unit cell})\right\}(6.023\times10^{23}\text{ atoms/mol})} \quad 5.07\text{ g/cm}^3$$

Niobium has an atomic radius of 0.1430 nm and a density of 8.57 g/cm^3. Determine whether it has an FCC or BCC crystal structure, the atomic weight of Niobium is 92.91 g/mol. which is the value provided in the problem statement. Therefore, Nb has a BCC crystal structure

4.12 In order to determine whether Nb has an FCC or a BCC crystal structure, we need to compute its density for each of the crystal structures. For FCC, n = 4, and $a = 2R\sqrt{2}$ (Equation 4.1). Also, from Figure 2.6, its atomic weight is 92.91 g/mol. Thus, for FCC (employing Equation 4.5)

$$\rho = \frac{nA_{Nb}}{a^3 N_A} = \frac{nA_{Nb}}{(2R\sqrt{2})^3 N_A} = \frac{(4\text{ atoms/unit cell})(92.91\text{ g/mol})}{\left\{\left[(2)(1.43\times10^{-8}\text{ cm})(\sqrt{2})\right]^3/(\text{unit cell})\right\}(6.023\times10^{23}\text{ atoms/mol})} = 9.33\text{ g/cm}^3$$

For BCC, n = 2, and $a = \frac{4R}{\sqrt{3}}$ (Equation 4.3), thus

$$\rho = \frac{nA_{Nb}}{\left(\frac{4R}{\sqrt{3}}\right)^3 N_A} \quad \rho = \frac{(2\text{ atoms/unit cell})(92.91\text{ g/mol})}{\left\{\left[\frac{(4)(1.43\times10^{-8}\text{ cm})}{\sqrt{3}}\right]^3/(\text{unit cell})\right\}(6.023\times10^{23}\text{ atoms/mol})} = 8.57\text{ g/cm}^3$$

The unit cell for uranium has orthorhombic symmetry, with *a*, *b*, and *c* lattice parameters of 0.286, 0.587, and 0.495 nm, respectively. If its density, atomic weight, and atomic radius are 19.05 g/cm^3, 238.03 g/mol, and 0.1385 nm, respectively, compute the atomic packing factor.

4.14 In order to determine the APF for U, we need to compute both the unit cell volume (V_C) which is just the product of the three unit cell parameters, as well as the total sphere volume (V_S) which is just the product of the volume of a single sphere and the number of spheres in the unit cell (n). The value of n may be calculated from Equation 4.5 as

$$n = \frac{\rho V_C N_A}{A_U} = \frac{(19.05\ \text{g/cm}^3)(2.86)(5.87)(4.95)(\times 10^{-24}\ \text{cm}^3)(6.023 \times 10^{23}\ \text{atoms/mol})}{238.03\ \text{g/mol}} = 4.01\ \text{atoms/unit cell}$$

Therefore

$$\text{APF} = \frac{V_S}{V_C} = \frac{(4)\left(\frac{4}{3}\pi R^3\right)}{(a)(b)(c)} = \frac{(4)\left[\frac{4}{3}(\pi)(1.385\text{Ź}x\ 10^8\ \text{cm})^3\right]}{(2.86)(5.87)(4.95)(x\text{Ź}10^{24}\ \text{cm}^3)} = 0.536$$

Determine the total void volume (cm^3 /mole) for gold (Au) at 27ºC; make the hard-sphere approximation in your calculation, and use data provided in the periodic table.

First determine the packing density for Au, which is FCC; then relate it to the molar volume given in the periodic table.

$$\text{packing density} = \frac{\text{volume of atoms/unit cell}}{\text{volume of unit cell}} = \frac{\frac{16\pi r^3}{3}}{a^3} = \frac{16\pi r^3}{3a^3}$$

$$\text{packing density} = \frac{16\pi r^3}{3 \times 16\sqrt{2}r^3} = \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$$

$$\text{void volume} = 1 - \text{packing density} = 26\%$$

From the packing density (74%) we recognize the void volume to be 26%. Given the molar volume as 10.3 cm^3/mole, the void volume is:

$$0.26 \times 10.3\ \text{cm}^3/\text{mole} = 2.68\ \text{cm}^3/\text{mole}$$

Determine the atomic radius of Mo. Given that atomic weight is 95.94 g/mol and density of Mo is 10.2 g/cm^3.

Mo: atomic weight = 95.94 g/mole

$\rho = 10.2\ g/cm^3$

BCC, so n = 2 atoms/unit cell

$$a^3 = \frac{(95.94\ g/mole)(2\ atoms/unit\ cell)}{(10.2\ g/cm^3)(6.023\times10^{23}\ atoms/mole)}\times10^{-6}\ \frac{m^3}{cm^3}$$

$$= 3.12\times10^{-29}\ m^3$$

$$a = 3.22\times10^{-10}\ m$$

For BCC, $a\sqrt{3} = 4r$, so $r = 1.39\times10^{-10}$ m

A metal is found to have BCC structure, a lattice constant of 3.31 Angstroms, and a density of 16.6 g/cm^3. Determine the atomic weight of the element.

BCC structure, so n = 2

$a = 3.31\ Å = 3.31 \times 10^{-10}$ m

$\rho = 16.6\ g/cm^3$

$$\frac{atomic\ weight}{\rho}\times10^{-6} = \frac{N_A}{n}\times a^3$$

$$atomic\ weight = \frac{(6.023\times10^{23}\ atoms/mole)\ (3.31\times10^{-10}\ m)^3}{(2\ atoms/unit\ cell)(10^{-6}\ m^3/cm^3)}\times16.6\ g/cm^3$$

$= 181.3$ g/mole

Session #15: Homework Solutions

Problem #1

Iron ($\rho = 7.86$ g/cm^3) crystallizes in a BCC unit cell at room temperature. Calculate the radius of an iron atom in this crystal. At temperatures above 910°C iron prefers to be FCC. If we neglect the temperature dependence of the radius of the iron atom on the grounds that it is negligible, we can calculate the density of FCC iron. Use this to determine whether iron expands or contracts when it undergoes transformation from the BCC to the FCC structure.

Solution

In BCC there are 2 atoms per unit cell, so $\frac{2}{a^3} = \frac{N_A}{V_{molar}}$, where $V_{molar} = A/\rho$; A is the atomic mass of iron.

$$\frac{2}{a^3} = \frac{N_A \times \rho}{A}$$

$$\therefore\ a = \left(\frac{2A}{N_A \times \rho}\right)^{\frac{1}{3}} = \frac{4}{\sqrt{3}} r$$

$$\therefore\ r = 1.24 \times 10^{-8} \text{ cm}$$

If we assume that change of phase does not change the radius of the iron atom, then we can repeat the calculation in the context of an FCC crystal structure, i.e., 4 atoms per unit cell and $a = 2\sqrt{2}r$.

$$\rho = \frac{4A}{N_A (2\sqrt{2}r)^3} = 8.60 \text{ g/cm}^3$$

FCC iron is more closely packed than BCC suggesting that iron contracts upon changing from BCC to FCC. This is consistent with the packing density calculations reported in lecture that give FCC as being 74% dense and BCC 68% dense. The ratio of the densities calculated here is precisely the same:

$$\frac{7.86}{8.60} = \frac{0.68}{0.74}$$

Problem #2

Determine the total void volume (cm^3/mole) for gold (Au) at 27°C; make the hard-sphere approximation in your calculation, and use data provided in the periodic table.

Solution

First determine the packing density for Au, which is FCC; then relate it to the molar volume given in the periodic table.

$$\text{packing density} = \frac{\text{volume of atoms/unit cell}}{\text{volume of unit cell}} = \frac{\frac{16\pi r^3}{3}}{a^3} = \frac{16\pi r^3}{3a^3}$$

$$\text{packing density} = \frac{16\pi r^3}{3 \times 16\sqrt{2} r^3} = \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$$

void volume = 1 − packing density = 26%

From the packing density (74%) we recognize the void volume to be 26%. Given the molar volume as 10.3 cm^3/mole, the void volume is:

$$0.26 \times 10.3 \text{ cm}^3 / \text{ mole} = 2.68 \text{ cm}^3 / \text{ mole}$$

Problem #3

Determine the atomic (metallic) radius of Mo. Do not give the value listed in the periodic table; calculate it from other data given.

Solution

Mo: atomic weight = 95.94 g/mole

ρ = 10.2 g/cm^3

BCC, so n = 2 atoms/unit cell

$$a^3 = \frac{(95.94 \text{ g/mole})(2 \text{ atoms/unit cell})}{(10.2 \text{ g / cm}^3)(6.023 \times 10^{23} \text{ atoms/mole})} \times 10^{-6} \frac{\text{m}^3}{\text{cm}^3}$$

$$= 3.12 \times 10^{-29} \text{ m}^3$$

$$a = 3.22 \times 10^{-10} \text{ m}$$

For BCC, $a\sqrt{3} = 4r$, so $r = 1.39 \times 10^{-10}$ m

Problem #4

A metal is found to have BCC structure, a lattice constant of 3.31 Å, and a density of 16.6 g/cm^3. Determine the atomic weight of this element.

Solution

BCC structure, so n = 2

a = 3.31 Å = 3.31 x 10^{-10} m

ρ = 16.6 g/cm^3

$$\frac{\text{atomic weight}}{\rho} \times 10^{-6} = \frac{N_A}{n} \times a^3$$

$$\text{atomic weight} = \frac{(6.023\times10^{23}\ \text{atoms/mole})\ (3.31\times10^{-10}\ \text{m})^3}{(2\ \text{atoms/unit cell})(10^{-6}\ \text{m}^3/\text{cm}^3)}\times16.6\ \text{g/cm}^3$$

$$= 181.3\ \text{g/mole}$$

Problem #5

At 100°C copper (Cu) has a lattice constant of 3.655 Å. What is its density at this temperature?

Solution

Cu is FCC, so n = 4

$a = 3.655\ \text{Å} = 3.655 \times 10^{-10}\ \text{m}$

atomic weight = 63.55 g/mole

$$\frac{\text{atomic weight}}{\rho}\times10^{-6} = \frac{N_A}{n}\times a^3$$

$$\rho = \frac{(63.55\ \text{g/mole})(4\ \text{atoms/unit cell})}{(6.023\times10^{23}\ \text{atoms/mole})(3.655\times10^{-10}\ \text{m}^3)} = 8.64\ \text{g/cm}^3$$

Problem #6

Determine the second-nearest neighbor distance for nickel (Ni) (in pm) at 100° C if its density at that temperature is 8.83 g/cm^3.

Solution

Ni: n = 4

atomic weight = 58.70 g/mole

$\rho = 8.83\ \text{g/cm}^3$

For a face−centered cubic structure, the second nearest neighbor distance equals "a" (see LN4−11).

$$\frac{\text{atomic weight}}{\rho}\times10^{-6} = \frac{N_A}{n}\times a^3$$

$$a^3 = \frac{(58.70\ \text{g/mole})(10^{-6}\ \text{m}^3/\text{cm}^3)(4\ \text{atoms /unit cell})}{(6.023\times10^{23}\ \text{atoms / mole})(8.83\ \text{g / cm}^3)}$$

$$= 4.41\times10^{-29}\ \text{m}^3$$

$$a = 3.61\times10^{-10}\ \text{m}\times\frac{10^{12}\ \text{pm}}{\text{m}} = 3.61\times10^{2}\ \text{pm}$$

Problem #7

Determine the highest linear density of atoms (atoms/m) encountered in vanadium (V).

Solution

V: atomic weight = 50.94 g/mole

$\rho = 5.8\ g/cm^3$

BCC, so n = 2

The highest density would be found in the [111] direction. To find "a":

$$\frac{\text{atomic weight}}{\rho} = a^3 \frac{N_A}{n} \rightarrow a^3 = \frac{50.94 \times 2}{5.8 \times 6.023 \times 10^{23}}$$

$$a = 3.08 \times 10^{-8}\ cm = 3.08 \times 10^{-10}\ m$$

The length in the [111] direction is $a\sqrt{3}$, so there are:

$$2\ \text{atoms} / a\sqrt{3} = 2\ \text{atoms}/(3.08 \times 10^{-10}\ m \times \sqrt{3})$$

$$= 3.75 \times 10^9\ \text{atoms/m}$$

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General unit cell problems

Go to the body-centered cubic problems

Go to the face-centered cubic problems

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Problem #1: Many metals pack in cubic unit cells. The density of a metal and length of the unit cell can be used to determine the type for packing. For example, sodium has a density of 0.968 g/cm^3 and a unit cell side length (a) of 4.29 Å

a. How many sodium atoms are in 1 cm^3?
b. How many unit cells are in 1 cm^3?
c. How many sodium atoms are there per unit cell?

Solution:

1) Calculate the average mass of one atom of Na:

$22.99 \text{ g mol}^{-1} \div 6.022 \times 10^{23} \text{ atoms mol}^{-1} = 3.82 \times 10^{-23} \text{ g/atom}$

2) Determine atoms in 1 cm^3:

$0.968 \text{ g} / 3.82 \times 10^{-23} \text{ g/atom} = 2.54 \times 10^{22} \text{ atoms in 1 cm}^3$

3) Determine volume of the unit cell:

$(4.29 \times 10^{-8} \text{ cm})^3 = 7.89 \times 10^{-23} \text{ cm}^3$

4) Determine number of unit cells in 1 cm^3:

$1 \text{ cm}^3 / 7.89 \times 10^{-23} \text{ cm}^3 = 1.27 \times 10^{22} \text{ unit cells}$

5) Determine atoms per unit cell:

$2.54 \times 10^{22} \text{ atoms} / 1.27 \times 10^{22} \text{ unit cells} = 2 \text{ atoms per unit cell}$

Problem #2: Metallic iron crystallizes in a type of cubic unit cell. The unit cell edge length is 287 pm. The density of iron is 7.87 g/cm3. How many iron atoms are there within one unit cell?

Solution:

1) Calculate the average mass of one atom of Fe:

$55.845 \text{ g mol}^{-1} \div 6.022 \times 10^{23} \text{ atoms mol}^{-1} = 9.2735 \times 10^{-23} \text{ g/atom}$

2) Determine atoms in 1 cm^3:

$7.87 \text{ g} / 9.2735 \times 10^{-23} \text{ g/atom} = 8.4866 \times 10^{22} \text{ atoms in 1 cm}^3$

3) Determine volume of the unit cell:

$287 \text{ pm} \times (1 \text{ cm} / 10^{10} \text{ pm}) = 2.87 \times 10^{-8} \text{ cm}$

$(2.87 \times 10^{-8}\ cm)^3 = 2.364 \times 10^{-23}\ cm^3$

4) Determine number of unit cells in 1 cm^3:

$1\ cm^3 / 2.364 \times 10^{-23}\ cm^3 = 4.23 \times 10^{22}$ unit cells

5) Determine atoms per unit cell:

8.4866×10^{22} atoms / 4.23×10^{22} unit cells = 2 atoms per unit cell

---

Problem #3: (a) You are given a cube of silver metal that measures 1.015 cm on each edge. The density of silver is 10.49 g/cm^3. How many atoms are in this cube?

Solution to a:

$(1.015\ cm)^3 \times (10.49\ g / cm^3) \times (1\ mole\ Ag / 107.9\ g) \times (6.023 \times 10^{23}$ atoms / 1 mole) = 6.12×10^{22} atoms Ag

(b) Because atoms are spherical, they cannot occupy all of the space of the cube. The silver atoms pack in the solid in such a way that 74% of the volume of the solid is actually filled with the silver atoms. Calculate the volume of a single silver atom.

Solution to b:

$(1.015\ cm)^3 \times 0.74 = 0.774\ cm^3$ filled by Ag atoms
$0.774\ cm^3 / (6.12 \times 10^{22}$ atoms) = $1.26 \times 10^{-23}\ cm^3$ / Ag atom

(c) Using the volume of a silver atom and the formula for the volume of a sphere, calculate the radius in angstroms of a silver atom.

Solution to c:

$V = (4/3)\ \pi\ r^3$
$r^3 = V / (4/3)\ \pi = [(1.26 \times 10^{-23}\ cm^3)\ (3)] / [(4)\ (3.14159)] = 3.008 \times 10^{-24}\ cm^3$

$r = 1.4435 \times 10^{-8}$ cm = 1.44 Å

Problem #4: Many metals pack in cubic unit cells. The density of a metal and length of the unit cell can be used to determine the type for packing. For example, gold has a density of 19.32 g/cm^3 and a unit cell side length of 4.08 Å. (1 Å = 1×10^{-8} cm.)

(a) How many gold atoms are in exactly 1 cm^3?
(b) How many unit cells are in exactly 1 cm^3?
(c) How many gold atoms are there per unit cell?
(d) The atoms/unit cell suggests that gold packs as a (i) simple, (ii) body-centered or (iii) face-centered unit cell.

Solution:

1) Part a:

19.32 g / 197.0 g/mol = 0.098071 mol

0.098071 mol times 6.022×10^{23} atoms/mol = 5.9058×10^{22} atoms

2) Part b:

4.08 Å = 4.08 x 10^{-8} cm

1 cm divided by 4.08 x 10^{-8} cm = 24509804 (this is how many 4.08 Å segments in 1 cm)

24509804 cubed = 1.47238 x 10^{22} unit cells

3) Part c:

5.9058 x 10^{22} atoms / 1.47238 x 10^{22} unit cells = 4 atom/unit cell

4) Part d:

face-centered

Problem #5: A metal nitride has a nitrogen atom at each corner and a metal atom at each edge. Which is the empirical formula for this nitride?

a. Ba_3N_2
b. Na_3N
c. AlN
d. Ti_3N_4

Solution:

A cube has eight corners and an atom at a corner is in eight different cubes; therefore 1/8 of an atom at each corner of a given cube. So:

1/8 times 8 = 1 total nitrogen atom in each cube

A cube has 12 edges and each edge is in 4 different cubes, so there is 1/4 of an atom in each individual cube. So:

1/4 times 12 = 3 total metal atoms in each cube

The only choice to fit the above criteria is answer choice b, Na_3N.

Problem #6: Calcium fluoride crystallizes with a cubic lattice. The unit cell has an edge of 546.26 pm and has a density of 3.180 g/cm^3. How many formula units must there be per unit cell?

Solution:

1) Convert pm to cm:

546.26 pm times (1 cm / 10^{10} pm) = 5.4626 x 10^{-8} cm

2) Determine volume of unit cell:

$(5.4626 \times 10^{-8}\ cm)^3 = 1.63 \times 10^{-22}\ cm^3$

3) Determine mass of CaF_2 in unit cell:

3.180 g/cm^3 times 1.63 x 10^{-22} cm^3 = 5.1835 x 10^{-22} g

4) Determine mass of one formula unit of CaF_2:

formula weight of CaF_2 = 78.074 g/mol

78.074 g/mol divided by 6.022×10^{23} formula units / mole = 1.2965×10^{-22} g

5) Determine number of formula units in one unit cell:

5.1835×10^{-22} g divided by 1.2965×10^{-22} g = 3.998

There are 4 formula units of CaF_2 per unit cell

Problem #7: Tungsten has an atomic radius of 137 pm and crystallizes in a cubic unit cell having an edge length d = 316 pm. What type of cubic unit cell does tungsten crystallize in?

Solution:

Let us assume the cell is face-centered. If this is the case, then this relationship should hold true:

$d^2 + d^2 = (4r)^2$

where r = the radius.

Please see a small discussion of this in problem #1 here.

Using 316 pm for d and 548 pm for 4r, we have this:

$316^2 + 316^2 \text{ ?=? } 548^2$

We find 199712 for the left and 300304 for the right, so the idea that tungsten is fcc fails.

For body-centered, please see problem #2 here for this equation:

$d^2 + (d\sqrt{2})^2 = (4r)^2$

$3d^2 = (4r)^2$

$3(316^2) \text{ ?=? } 548^2$

299568 = 300304

Due to the fact that these numbers are roughly equivalent, we can conclude that tungsten is being body-centered cubic.

Problem #8: What is the formula of the compound that crystallizes with Ba^{2+} ions occupying one-half of the cubic holes in a simple cubic arrangement of fluoride ions?

Solution:

We must consider two cubic unit cells, one with the barium ion and one without (this gives us one-half of the cubic holes filled).

Cell 1: 8 F atoms at the 8 vertices. Since each vertex is in a total of 8 cells, we have 1 F atom in the unit cell. The cubic hole in the middle of the cell is empty.

Cell 2: 8 F atoms at the 8 vertices. Since each vertex is in a total of 8 cells, we have 1 F atom in the unit cell. The cubic hole in the middle of the cell has a barium in it.

Total for the two cells: one Ba and two F

Formula: BaF_2

Problem #9: The radius of gold is 144 pm, and the density is 19.32 g/cm^3. Does gold crystallize in a face-centered cubic structure or a body-centered cubic structure?

Solution:

1) I will assume the unit cell is face-centered cubic. I will use that assumption and the atomic radii to calculate the volume of the cell. From there, I will use the fact that there are 4 atoms of gold in the unit cell to determine the density. The final step will be to compare it to the 19.32 value. Here is one face of a face-centered cubic unit cell:

2) Across the face of the unit cell, there are 4 radii of gold, hence 576 pm. Using the Pythagorean Theorem, we determine the edge length of the unit cell:

$d^2 + d^2 = 576^2$

d = 407.2935 pm

3) Let us convert the pm to cm:

4407.2935 pm times (1 cm / 10^{10} pm) = 4.072935×10^{-8} cm

4) The volume of the unit cell:

$(4.072935 \times 10^{-8}\ cm)^3 = 6.75651 \times 10^{-23}\ cm^3$

5) The mass of 4 gold atoms:

(196.96655 g/mol divided by 6.022×10^{23} atoms/mol) times 4 atoms = 1.308313×10^{-21} g

6) Let's see what density results:

$1.308313 \times 10^{-21}\ g / 6.75651 \times 10^{-23}\ cm^3 = 19.36\ g/cm^3$

We conclude that gold crystallizes fcc because we were able to reproduce the known density of gold.

7) Let's do the bcc calculation (which we know will give us the wrong answer). Here's an image showing what to do with the Pythagorean Theorem:

8) The rest of the calculation with minimal comment:

$d^2 + (d\sqrt{2})^2 = 576^2$

d = 332.55 pm

332.55 pm = 3.3255×10^{-8} cm

$(3.3255 \times 10^{-10}\ cm)^3 = 3.6776 \times 10^{-23}\ cm^3$

There are two atoms in a body-centered cubic.

(197 g/mol divided by 6.022×10^{23} atoms/mol) times 2 atoms = 6.5427×10^{-22} g

6.5427×10^{-22} g / 3.6776×10^{-23} cm^3 = 17.79 g/cm^3

Gold does not crystallize bcc because bcc does not reproduce the known density of gold.

Problem #10: Avogadro's number has been determined by about 20 different methods. In one approach, the spacing between ions in an ionic substance is determined by using X-ray diffraction. X-ray diffraction of sodium chloride have shown that the distance between adjacent Na^+ and Cl^- ions is 2.819×10^{-8} cm. The density of solid NaCl is 2.165 g/cm^3. By calculating the molar mass to four significant figures, you can determine Avogadro's number. What value do you obtain?

Solution:

1) Imagine a cube with 4 Na and 4 Cl at adjacent vertices. I'll call it the reference cube.

There's going to be a twist and it involves how many Na and Cl are in the cube. Think about it before the reveal in the last step.

2) Determine the volume of the cube:

$(2.819 \times 10^{-8}\ cm)^3 = 2.2402 \times 10^{-23}\ cm^3$

3) Calculate the mass of NaCl inside the cube:

2.2402×10^{-23} cm^3 times 2.165 g/cm^3 = 4.85×10^{-23} g

4) The molar mass divided by the mass inside the cube equals Avogadro's Number. Here's where the twist comes into play.

Each Na and each Cl at a vertex of the reference cube is shared by a total of 8 cubes. (You may verify this on your own.) At any one vertex, there is 1/8 of a Na atom and 1/8 of a Cl atom inside the reference cube.

With the reference cube having 4 vertices of Na and 4 vertices of Cl, this means there is a total of 1/2 of a Na atom and 1/2 of a Cl atom inside the reference cube.

The "molar mass" of (1/2)NaCl is half of 58.443.

29.2215 g/mol divided by 4.85×10^{-23} g = 6.025×10^{23} mol^{-1}

Problem #11: Many metals pack in cubic unit cells. The density of a metal and length of the unit cell can be used to determine the type for packing. For example, platinum has a density of 21.45 g/cm^3 and a unit cell side length a of 3.93 Å. What is the atomic radius of platinum?

Solution:

1) Determine the volume of the unit cell:

$(3.93 \times 10^{-8}\ cm)^3 = 6.07 \times 10^{-23}\ cm^3$

Note that I converted from Å to cm. That's because of the density.

2) Determine the mass of Pt in one unit cell:

6.07×10^{-23} cm^3 times 21.45 g/cm^3 = 1.302×10^{-21} g

3) Determine number of Pt atoms in the given mass:

195.078 g/mol divided by 6.022 x 10^23 atom/mol = 3.2394×10^{-22} g/atom

1.302×10^{-21} g divided by 3.2394×10^{-22} g/atom = 4 atoms

I did the above calculations in order to determine if the unit cell was face-centered or body-centered. The answer of 4 atoms in the unit cell tells me that it is face-centered. I now know what to do to determine the atomic radius. To do so, I will use the Pythagorean Theorem. (See Problem #9 for an image illustrating a face-centered cubic.)

4) Solve the Pythagorean Theorem:

$d^2 + d^2 = (4r)^2$ (where r is the radius of the Pt atom. Four of them span the hypotenuse.)

$3.93^2 + 3.93^2 = 16r^2$

$r^2 = 30.8898 / 16 = 1.9306125$

r = 1.39 Å

Problem #12: The density of TlCl(s) is 7.00 g/cm^3 and that the length of an edge of a unit cell is 385 pm, (a) determine how many formula units of TlCl there are in a unit cell. Based on your answer for the number of formula units of TlCl(s) in a unit cell, (b) how is the unit cell of TlCl(s) likely to be structured?

Solution to (a):

1) Get the volume in cm:

$$(385 \text{ pm})\ (100 \text{ cm} / 10^{12} \text{ pm}) = 3.85 \times 10^{-8} \text{ cm}$$

2) Calculate the volume of the unit cell:

$$(3.85 \times 10^{-8} \text{ cm})^3 = 5.7066625 \times 10^{-23} \text{ cm}^3$$

3) Calculate the mass of TlCl in one unit cell:

$$(7.00 \text{ g/cm}^3)\ (5.7066625 \times 10^{-23} \text{ cm}^3) = 3.99466375 \times 10^{-22} \text{ g}$$

4) Determine how many moles of TlCl are in the unit cell:

$$3.99466375 \times 10^{-22} \text{ g} / 239.833 \text{ g/mol} = 1.6656022107 \times 10^{-24} \text{ mol}$$

5) Formula units of TlCl in the unit cell:

$$(1.6656022107 \times 10^{-24} \text{ mol})\ (6.022 \times 10^{23} \text{ mol}^{-1}) = 1.00$$

Solution to (b):

Body-centered cubic has two atoms per unit cell and a formula unit of TlCl has two atoms. One atom, say the chloride ion, occupies the center of the unit cell, while 1/8th of eight Tl^+ ions are present at each of the 8 vertices of the cube.

Face-centered cubic has 4 atoms per unit cell. The distribution of TlCl formula units into an fcc cell does not work.

Go to the body-centered cubic problems

Go to the face-centered cubic problems

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