

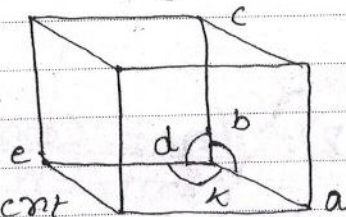
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# CRYSTAL STRUCTURE

Crystalline Solid: Crystalline Solid is that type of Solid in which there is a regular arrangement of atoms, molecules and particles within the Solid.

Amorphous Solid: A Solid is said to be amorphous if there is no regular arrangement of atoms, molecules, ions within the Solid.

Space lattice: Lattice is defined as a parallel net like arrangement of atoms provided that environment of any point is identical with the environment at any other point. The angle between the primitives  $a$ ,  $b$  and  $c$  is  $90^\circ$ .



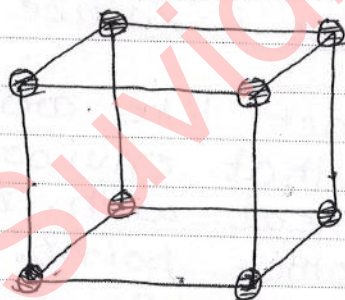
The regular arrangement of atoms, molecules and particles in three dimension space is called Space lattice.



Unit Cell: The Smallest portion of the complete space which is repeated again and again in different direction so as to produce complete (small) space lattice.

Types of Unit Cell:

1). Simple unit cell: In Simple unit cell atoms are present at the corners of each unit cell. An atom at unit cell is shared by all other eight atoms. Thus contribution of atom at corner of each unit cell is  $\frac{1}{8}$ .



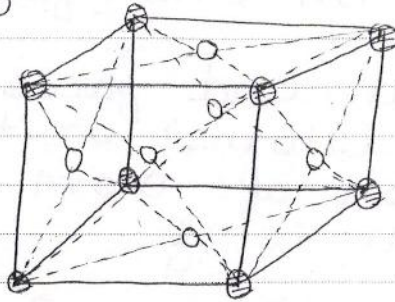
2). Face Centred Unit Cell: In face centred unit cell, atoms are present at face of each unit cell.

An atom present at face of each unit cell is shared by two unit cell. Thus contribution of atom



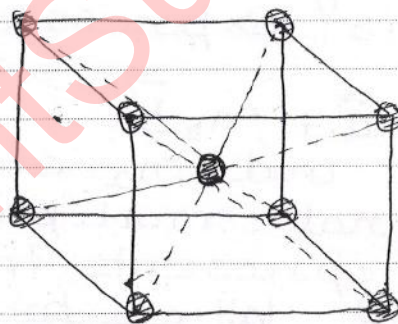
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at face of each unit cell =  $\frac{1}{2}$



3). Body Centred unit Cell: In body centred unit cell, atoms are present at the corners of unit cell as well as on the body of unit cell.

An atom at body of unit cell is not shared by other unit cell. Contribution of atom at the body of unit cell = 1



Notes

4). End Face (edge) Centred unit Cell:

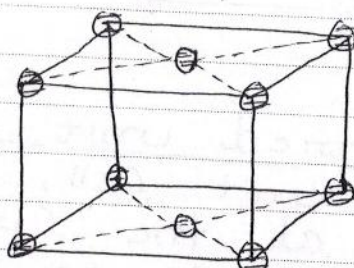
In end face centred unit cell, atom

Birthday / Anniversary



are present at corners of unit cell as well as on end faces of unit cell.

An atom at end faces is shared by four other (atoms) unit cell. Thus, contribution of atom at end face of unit cell is  $\frac{1}{4}$ .

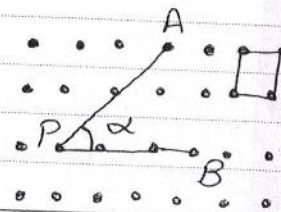


### TRANSLATIONAL VECTOR (operator):

The position vector of lattice points in two dimensional space by choosing any other lattice point as origin is expressed as:

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b}$$

where  $n_1$  and  $n_2$  are the integral multiple which represents the number of lattice points along PA and PB axis.



The position vector of lattice points in three dimensional space is



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|        | 29 | 30 |    |    |    |    |    |

is expressed by translational operator

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$$

where  $a, b$  and  $c$  are the primitives along  $p_A, p_B$  and  $p_C$  (in three dimension) axis.

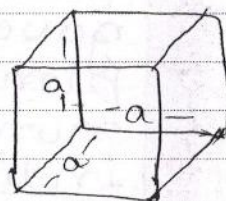
Lattice Constant 'a' ✓ DO

let us consider a Cubic Crystal of lattice constant 'a'. Volume of each unit cell =  $a^3$ .

let  $\rho$  be density of the crystal under consideration.

then, mass of each unit cell =  $a^3 \rho$  -(1)

Let  $M$  be the molecular weight and 'N' (no. of molecules per kg mole of substance) be the avagadro's number.



Mass of each molecule =  $\frac{M}{N}$

If  $n$  be total number of molecule the mass of substance =  $\frac{nM}{N}$  -(2)

Equating ① and ②

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



8.00

$$a = \left( \frac{nM}{\rho \cdot N} \right)^{1/3}$$

9.00

'a' is lattice constant.

10.00

## Lattice plane and Miller Indices

11.00

The plane passing through lattice is called lattice plane.

12.00

Lattice plane can be drawn in different number of ways for example (a), (b), (c)

1.00

2.00

3.00

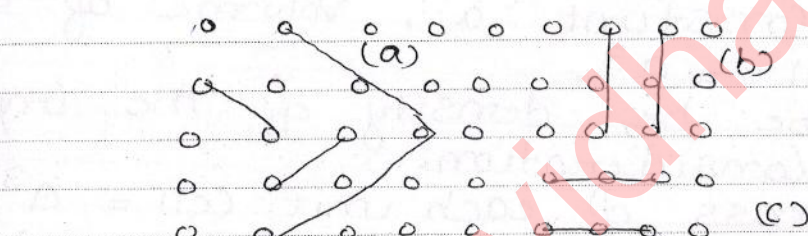
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Now, problem is to designate the plane in the crystal. So, Miller gave a method to designate a plane in a crystal by three numbers  $h, k, l$  called Miller indices.

Miller indices are the three smallest possible integer values which have same ratio as the reciprocal of the intercepts concerned on three axis.

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Week 45

Day 311 • 054

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Saturday

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8.00 Procedure for drawing indices:

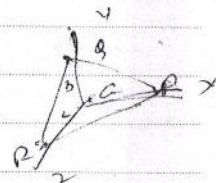
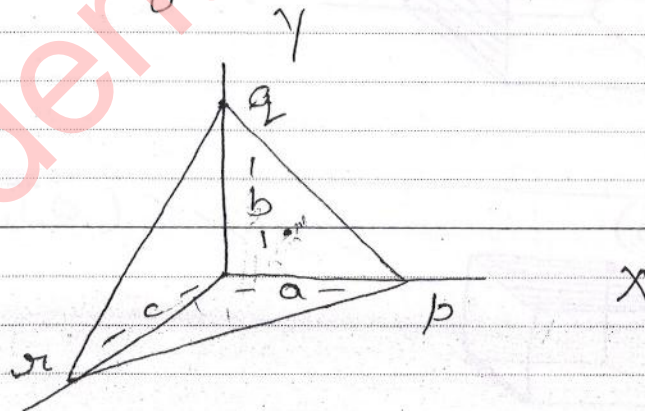
9.00 1). First of all find the intercepts concerned on three axis in the ratio of  $pa$ ,  $qb$  and  $rc$  along  $x$ - $y$  and  $z$ -axis.

11.00 2). Convert these intercepts into integral multiple by dividing the fundamental vectors to each intercepts.

12.00 3). Take the reciprocal of the intercepts as:

$$1.00 \quad \frac{1}{p} : \frac{1}{q} : \frac{1}{r}$$

4). Convert these intercepts into whole number by multiplying a number obtained after taking L.C.M of denominators.



Notes

Birthday / Anniversary

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November 2009

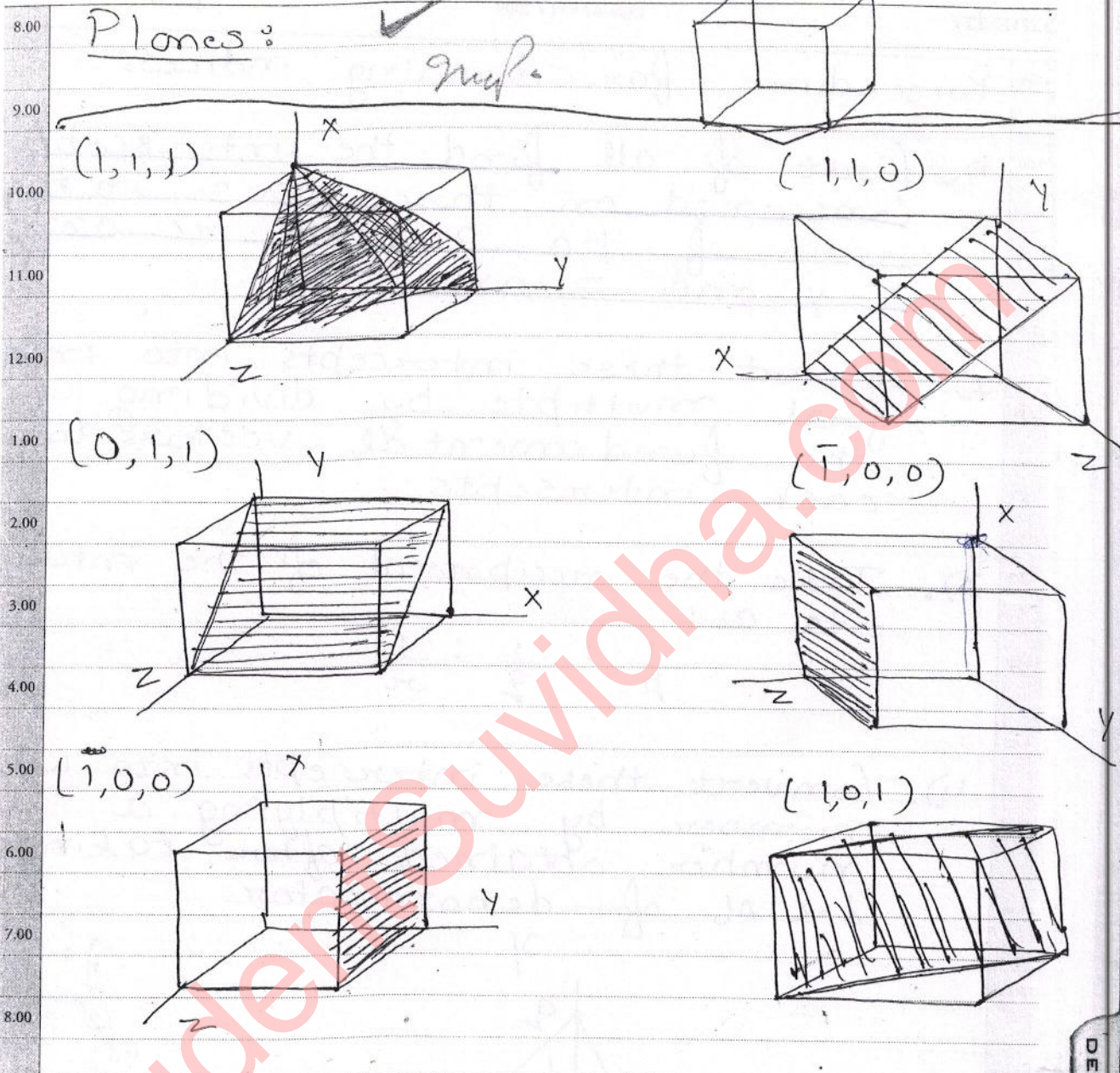
Week 45

Day 312 • 053

Date 08 • 11 • 2009

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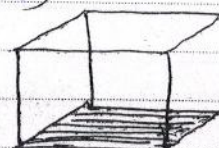
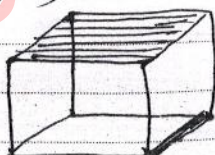
Sunday



Notes

(0,1,0)

(0,1,0)



Birthday / Anniversary



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## Seperation between lattice plane

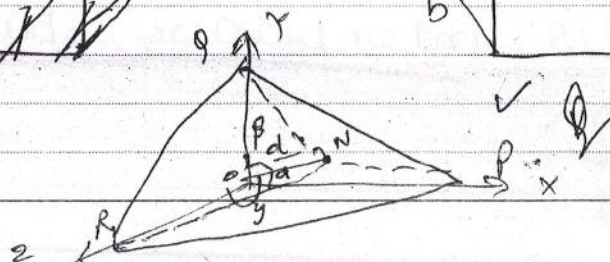
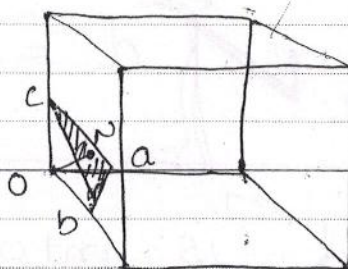
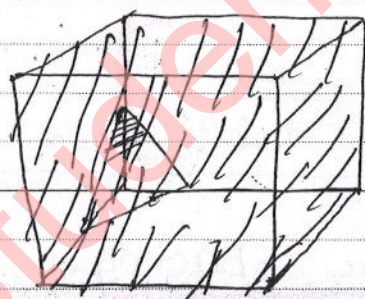
Consider a Crystal ABC having Miller indices  $(h, k, l)$ . Draw ON perpendicular to this plane. ON represents the interplanar spacing  $d$ . The angle between the coordinate axis is  $\alpha$ ,  $\beta$  and  $\gamma$ .

Intercepts concerned on three axis is  $OA = pa$ ,  $OB = qa$  and  $OC = ra$  but the miller indices remain same. Miller indices can be written in terms of intercepts as:

$$h = \frac{1}{p}, \quad k = \frac{1}{q} \quad \text{and} \quad l = \frac{1}{r}$$

$$\text{or } p = \frac{1}{h}, \quad q = \frac{1}{k} \quad \text{and} \quad r = \frac{1}{l}$$

So,  $OA = \frac{a}{h}$ ,  $OB = \frac{a}{k}$  and  $OC = \frac{a}{l}$





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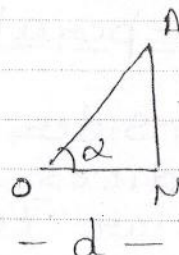
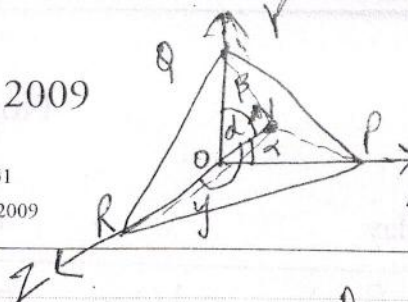
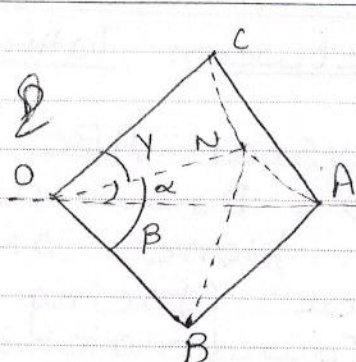
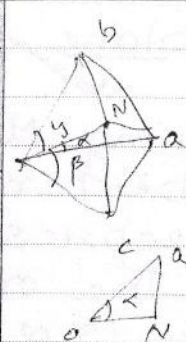
Week 46

Day 314 • 051

Date 10 • 11 • 2009

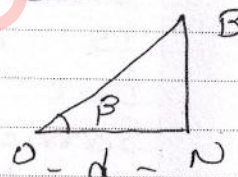
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Tuesday

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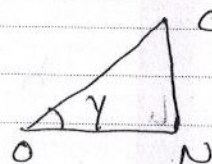


In  $\triangle ONA$ ,  $\cos \alpha = \frac{d}{OA} = \frac{dh}{a} \quad (1)$

In  $\triangle ONB$ ,  $\cos \beta = \frac{dk}{a}$



In  $\triangle ONC$ ,  $\cos \gamma = \frac{dl}{a}$



Using cosine theorem,

$$\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = \frac{d^2 h^2}{a^2} + \frac{d^2 k^2}{a^2} + \frac{d^2 l^2}{a^2} = \frac{d^2 (h^2 + k^2 + l^2)}{a^2}$$

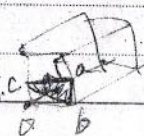
$$h^2 + k^2 + l^2 = \frac{a^2}{d^2} (h^2 + k^2 + l^2)$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Notes

$d$  is interplanar spacing.

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$$\frac{d^2 h^2}{a^2} + \frac{d^2 k^2}{a^2} + \frac{d^2 l^2}{a^2} = \frac{d^2 (h^2 + k^2 + l^2)}{a^2}$$



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| NOV 09 | 29 | 30 |    |    |    |    |    |

## Bonding in Solid:

When two atoms are brought near to each other then electrons re-arrange to acquire stable configuration. Thus, rearrangement of electron causes various types of bonding in Solids.

### Ionic Bonding:

Crystal in which ionic bonding is present is called ionic crystal. Crystals are not pure element but the compound of  $\text{NaCl}$ ,  $\text{KCl}$  etc.

When two different atoms are brought near to each other then if one atom has low ionisation energy so that it can lose electron easily and another atom has high electron affinity so that it can gain electron easily, an ionic bond is formed between the atom by transfer of electron.

Notes For ~~ex~~ example, Consider a  $\text{NaCl}$  crystal. Sodium atom has one electron



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Thursday

in Valence Shell, its electronic configuration is 2, 8, 1. So it is ready to lose one electron and Chlorine atom has Seven electrons in valence shell so it easily gains one electron.

When Sodium and chlorine atom are brought near to each other the electron is transferred from Sodium to chlorine atom as,



Due to strong electrostatic force of attraction, an ionic bond is formed.

### Covalent Bonding

Covalent bond is formed between atoms of same element or different element by sharing of valence electron. Here it should be remembered that electrons are not transferred between atoms but sharing of valence electron takes place.

Notes

For example, Consider  $\text{Cl}_2$  atom. Chlorine has Seven valence electrons in outermost shell. So, it is ready to gain one valence electron.

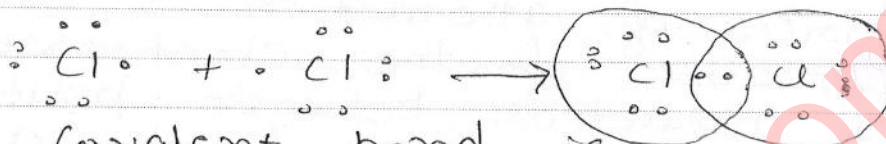
Birthday / Anniversary



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to acquire Stable Configuration, Some as the case with another Chlorine atom.

These two Chlorine atom Shares the electrons to Complete their octet. as;



Hence, Covalent bond is formed between chlorine atoms.

### Metallic Bonding:

In metal, valence electrons are mobile and are not bounded to particular atom. These valence electrons are free to move through out the whole volume of metal.

These free electrons and valence electrons form a cloud of electrons. Thus, atom may be regarded as array of closely packed ion or positive ion core immersed in the electron gas. There exists a strong force of attraction between the positive ion core and electron gas and metallic bond is formed when attraction (this) exceeds the mutual repulsion of electron in that gas.

Notes

Birthday / Anniversary



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14

Saturday

## Molecular Bonding:

Besides the force of attraction due to ionic, covalent and molecular there exists a weak force called London forces. London wall forces of attraction is caused because of the electrostatic force of attraction between positively charged nucleus of one atom with negatively charged electron of other atom.

There exists a weak repulsive force between negatively charged electron of one atom and negatively charged electron of other atom, or positively charged nucleus of one atom with positively charged nucleus of other. Thus, molecular bonding is formed due to weak London wall forces. For example: Noble gases have their octet completely filled so there is no possibility of the re-arrangement of electrons. Hence, noble gases are monoatomic at ordinary temperature and pressure. But these

Notes

conditions condensed at low temp, such condensation of noble gas is not possible if London wall forces are not present.

Birthday / Anniversary



15

Sunday

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BRAGG LAW:

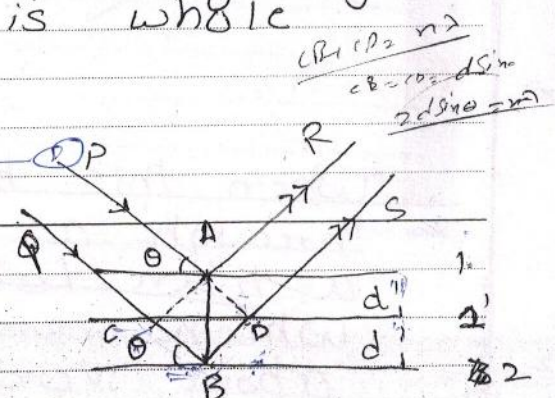
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Let us consider Set of parallel lattice plane of Crystal Separated by  $d$ . Let a beam of X-ray PA of wavelength  $\lambda$  incident upon these plane at angle  $\theta$  in direction AB at atom A from plane 1. Another beam of X-ray QB of wavelength  $\lambda$  incident on angle  $\theta$  at plane 2 in direction BC. ~~Two~~ two beams are reflected in direction AR and BS. Draw two perpendiculars AC and BD on incident ray QB and reflected ray BS. These two rays have a path difference  $(CB + DB)$ . These two rays will be in phase or in different phase depends upon the path difference. Two reflected rays will be in phase and produces maximum spot of light if path difference is whole multiple of  $n\lambda$ .

$$CB + BD = n\lambda$$

But  $CB = BD = d \sin \theta$   
(from fig.)

$$[2d \sin \theta = n\lambda]$$



Birthday / Anniversary



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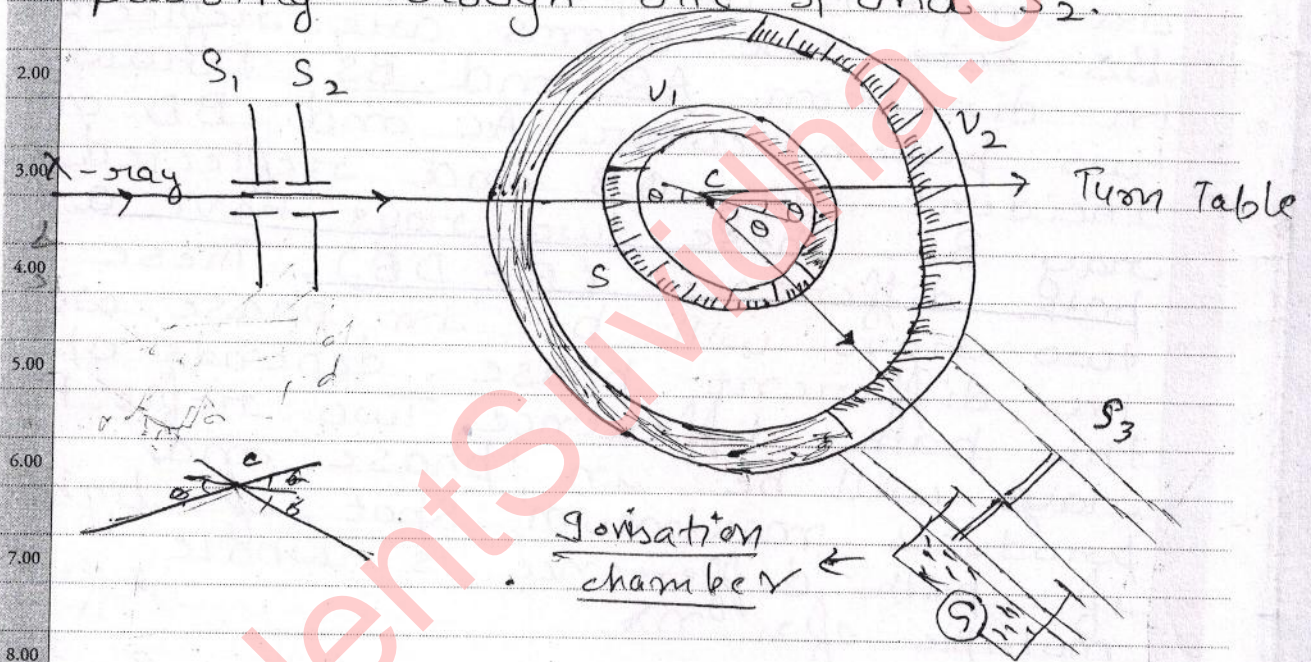
Monday

where  $n = 1, 2, 3, \dots$  for 1st, 2nd and  $n^{\text{th}}$  order maxima

This relation is called Bragg law.

Experimental method of bragg law.

The x-ray are produced from the x-ray tube narrowed to obtain a fine pencil like beam after passing through slit  $S_1$  and  $S_2$ .

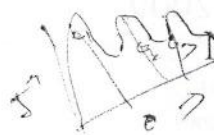


When this beam is allowed to pass through a crystal  $C$  mounted on a turn table of spectrometer, which is capable of rotation about vertical axis passing through

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the Centre. The rotation of turn table can be read from the Circular Scale S. Then the beam is allowed to pass through ionisation chamber mounted on movable arm of spectrometer. The position of the chamber can be read by second Vernier  $V_2$ . Now, reflected ray will enter into ionisation chamber only when turn table of spectrometer and ionisation chamber is linked in such a way that when turn table is rotated by angle  $\theta$  then chamber is rotated by angle  $2\theta$ . When beam enters into ionisation chamber, ionisation of gas takes place and two ion pairs are produced which moves to the respective electrode and current flows into the circuit which can be measured with help of galvanometer G.

The ionisation current can be determined by different value of glancing angle  $\theta$ . It is found that at particular glancing angle  $\theta$ , the intensity of ionisation current increases abruptly.

From Bragg law;



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Date 18 • 11 • 2009

18

Wednesday

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5.00

6.00

7.00

8.00

9.00

10.00

11.00

12.00

1.00

2.00

3.00

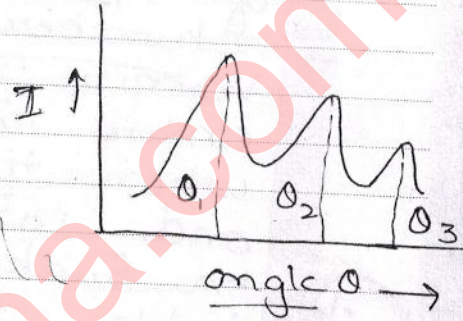
4.00

for 1st order Spectrum,  $2d \sin \theta_1 = \lambda$   
 for 2nd order Spectrum,  $2d \sin \theta_2 = 2\lambda$   
 for 3rd order Spectrum,  $2d \sin \theta_3 = 3\lambda$

$\therefore \sin \theta_1 : \sin \theta_2 : \sin \theta_3 = 1 : 2 : 3$

Graph is plotted between glancing angle  $\theta$  and ionisation current.

Thus, X-ray are reflected just like a ordinary light.



### Powder Method:

X-ray are allowed to pass through filter F, that absorbs all type of wavelength except one so we get monochromatic beam of X-ray.

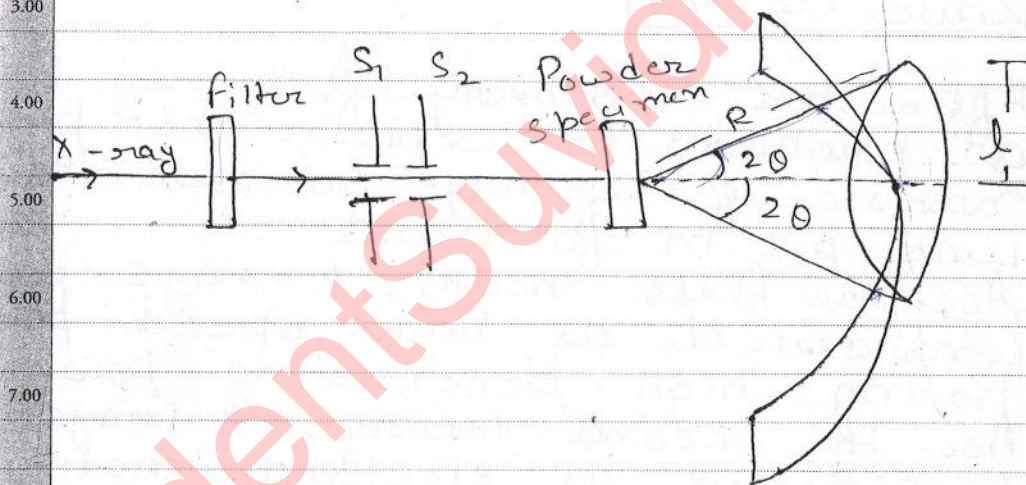
This beam is allowed to pass through Slits  $S_1$  and  $S_2$  to obtain a fine pencil like beam, which falls on powder specimen C placed at the Centre of drum shaped Cassette with photographic film at the inner circumference.

The basic principle of powder method is that it contains millions of microcrystals that



|        | S  | M  | T  | W  | T  | F  | S  |
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|        | 8  | 9  | 10 | 11 | 12 | 13 | 14 |
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|        | 29 | 30 |    |    |    |    |    |

have possible random orientations out of these there are some crystals whose lattice plane are so oriented to satisfy the bragg condition.  $2d \sin \theta = n\lambda$  reflection takes place at these plane and beam is reflected at angle  $2\theta$ . The parallel lattice plane with given spacing  $d$  and different value of  $n$  occurs at all position around axis of incident beam. The reflected beam produces a cone with semi vertical angle  $2\theta$ .



The intersection of different cone give ~~illumination~~ the series of concentric ring. Radius of these

Notes

Birthday / Anniversary



Concentric ring is used to calculate the glancing angle.  
If  $l$  is the radius of ring and  $R$  be radius of drum then  
glancing angle =  $\frac{\text{Arc of Circle}}{\text{radius}} = \frac{l}{R}$   
 $2\theta = \frac{l}{R}$ ,  $\theta = \frac{l}{2R}$

Acc. to Bragg law

$2d \sin \theta = n\lambda$   
From, here the inter planar spacing ' $d$ ' can be calculated.

### Laue Method

After the discovery of X-ray it remain a problem to explain the physical nature of X-rays so, two theory was put in forward.

Acc. to first theory, X-rays are considered as high speed particles having high penetrating power.

Acc. to second theory, X-rays are considered as electromagnetic waves of high frequency.

In order to test the wave nature it is essential that X-ray must produce either diffraction pattern or interference pattern. These



|        | S  | M  | T  | W  | T  | F  | S  |
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|        | 22 | 23 | 24 | 25 | 26 | 27 | 28 |
|        | 29 | 30 |    |    |    |    |    |

8.00 Conditions are well known in case of light wave.

9.00 According to diffraction theory of grating, diffraction pattern is obtained when spacing between the line rule on grating should be in order of magnitude of wavelength of light used.

10.00 According to Lave, x-ray are produced from x-ray tube narrowed to obtain a fine pencil like beam which is allowed to pass through slits  $S_1$  and  $S_2$ . This beam then crosses NaCl crystal and emergent ray produces a diffraction pattern on the screen and produces a black spot at  $O$  and series of other spot in definite pattern about  $O$ . The pattern is subjected to a condition that x-rays should go directly through NaCl crystal and produces a diffraction pattern on screen with central spot at  $O$ .

8.00 But there are weak diffracted beams which don't go directly through NaCl crystal and produces a series of spot about  $O$ . Thus, production of diffraction pattern depends upon type of crystal used.

Notes

Birthday / Anniversary



| F  | S  |
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November 2009

Week 47

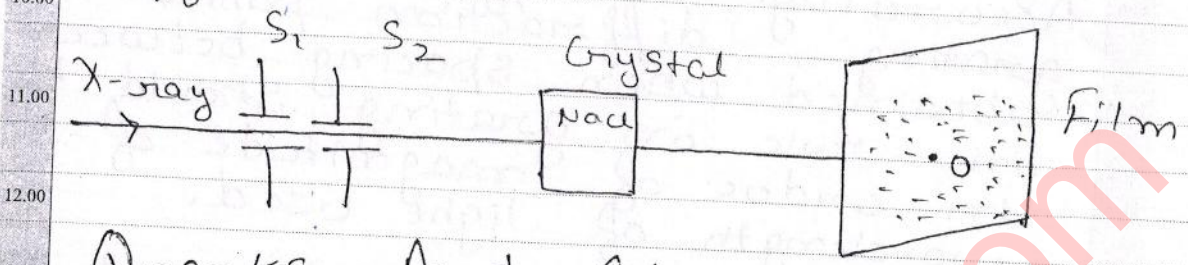
Day 326 • 039

Date 22 • 11 • 2009

22

Sunday

The Spots on the photographic film is called Laue spots and diffraction pattern is called Laue diffraction.



## Quarks And Gluons

Quarks are the fundamental particles that are constituents of proton, neutron and other hadrons. It is denoted by  $q$  and carries the fractional charge.

Types of quarks:

- 1) upquarks ( $u$ )
- 2) downquarks ( $d$ )
- 3) Strange quarks ( $s$ )
- 4) top quarks ( $t$ )
- 5) bottom quarks ( $b$ )
- 6) Charmed quarks ( $c$ )

Proton is made up of two upquark and one downquark.

Gluons: Gluons are the exchange particles which are responsible for the strong nuclear forces.



|        | S  | M  | T  | W  | T  | F  | S  |
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|        | 22 | 23 | 24 | 25 | 26 | 27 | 28 |
|        | 29 | 30 |    |    |    |    |    |

They binds quarks together to form a proton. Gluons are generally assumed to have zero electrical charge and zero mass. Gluons generates colour charge for quarks and have limited range.

### DEFECT :

Crystal is said to be perfect if there is regular arrangement of atoms, molecules and ions within the solid. If there is no regular arrangement of atoms then there may be defect in crystal.

Since, a defect can be of many types but important type of defect can be point defect.

Point defect can be caused due to presence of impurity atom or matrix atom in wrong place in crystal. It can be caused in two ways:

1. Impurity.

Impurity present in the crystal can cause the defect in the crystal.

It fits in structure into ways:

a) impurity atom may occupy a position normally occupied by central atom. defect is called Substitutional Impurity.



|        |    |    |    |    |    |    |    |
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|        | 27 | 28 | 29 | 30 | 31 |    |    |

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Week 48

Day 328 • 037

Date 24 • 11 • 2009

24

Tuesday

b) Impurity atom may lodge into unfilled spaces as voids are interstices called as interstitial impurity.

2). Vacancy —

If vacancy is present in the crystal then crystal is not perfect.

- If the atom leaves its site and dissolved interstitially into the structure, it is called Frenkel defect.

- Vacancy may also occur if an atom is missing from its lattice site, called Schottky defect.

(Imp.)

Concentration of Schottky defect: (19)

Let us consider a ideal crystal having equal number of positively charged ions and negative ions. Let  $N$  be the total no. of ions and  $n$  be total cation and anion Vacancy.

Notes

In order to calculate conc. of Schottky defect first of all calculate free energy.  $F = U - TS$  and for this calculate value of  $U$  and  $S$ .

Birthday / Anniversary



25

Wednesday

November 2009

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$$N_{C_n} = \frac{N!}{n!(N-n)!}$$

|        | S  | M  | T  | W  | T  | F  | S  |
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|        | 29 | 30 |    |    |    |    |    |

S can be calculated as ~~total~~ number of vacancy pairs is given by: which is to be selected at  $N$  sites

$$N_{C_n} = \frac{N!}{n!(N-n)!} \quad \text{--- (1)}$$

Total Vacancy pairs can be determined by Squaring above equation (1). This because [no. of cation vacancy = no. of anion vacancy.] ~~Shott Key defect~~

$$W = \left[ \frac{N!}{n!(N-n)!} \right]^2$$

$N! \approx \frac{N^N}{e^N}$   
 $\log W = 2 \log \left[ \frac{N!}{n!(N-n)!} \right]$   
 $\log W = 2 \log \left[ \frac{N^N}{e^N} \right]$

Acc. to Boltzmann Statistics:

$S = k_B \log W \rightarrow (2)$

If  $u$  is the energy required to produce a vacancy pair then total energy required to produce  $n$  vacancy pairs :-

$$U = nE \quad \text{--- (3)}$$

Now,  $F = U - TS$

$$F = nE - k_B T \log \left[ \frac{N!}{n!(N-n)!} \right]^2$$

Notes

$$F = nE - 2k_B T \log \frac{N!}{n!(N-n)!}$$

using Sterling approximation

Birthday / Anniversary



| S  | M  | T  | W  | T  | F  | S  |
|----|----|----|----|----|----|----|
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| 27 | 28 | 29 | 30 | 31 |    |    |

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Week 48

Day 330 • 035

Date 26 • 11 • 2009

$$\frac{E}{2k_B T} = \log \frac{N}{n}$$

$$e^{E/2k_B T} = \frac{N}{n}$$

26

Thursday

$\log x! = x \log x - x$

$$F = nE - 2k_B T [N \log N - N - n \log n + n - (N-n) \log(N-n) + (N-n)]$$

$$F = nE - 2k_B T [N \log N - n \log n - (N-n) \log(N-n)]$$

Differentiate w.r.t n

$$\frac{dF}{dn} = E - 2k_B T [0 - \frac{n}{n} - \log n - \frac{(N-n)}{N-n} - 1 + \log(N-n)]$$

$$\frac{dF}{dn} = E - 2k_B T [\log(N-n) - \log n]$$

We can calculate minimum to minimum no. of defect no max. to max

So,  $\left[ \frac{dF}{dn} = 0 \right]$

$$E = 2k_B T \log \left( \frac{N-n}{n} \right)$$

$$\frac{E}{2k_B T} = \log \frac{N-n}{n}$$

Since  $N \gg n$

$$e^{E/2k_B T} = \frac{N}{n}$$

Notes

$$n = N e^{-E/2k_B T}$$

Total no. of  
 Birthday / Anniversary  
 atomic vacancies

Total no. of  
 of ions

B. (its mass)  
 Centre



27

Friday

November 2009

Week 48

Day 331 • 034

Date 27 • 11 • 2009

| S  | M  | T  | W  | T  | F  | S  |
|----|----|----|----|----|----|----|
| 1  | 2  | 3  | 4  | 5  | 6  | 7  |
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| 15 | 16 | 17 | 18 | 19 | 20 | 21 |
| 22 | 23 | 24 | 25 | 26 | 27 | 28 |
| 29 | 30 |    |    |    |    |    |

NOV 09

10

8.00

## Concentration of Frankel defect *sub.*

9.00

10.00

11.00

12.00

1.00

2.00

3.00

4.00

5.00

6.00

7.00

8.00

Consider a crystal having equal no<sup>o</sup> of (+) charged ions and (-) charged ions. let  $N$  be no<sup>o</sup> of ions and  $n$  be the cation/anion vacancy. one Frankel defect constitutes one cation/anion vacancy or one interstitial ion.

In order to calculate the concentration of Frankel defect, first calculate free energy  $F = U - TS$ .  $S$  can be calculated in the sense that no<sup>o</sup> of cation/anion vacancy can be selected out of  $N$  ions as

$$N_c n = \frac{N!}{n! (N-n)!}$$

When one Frankel defect is produced, one interstitial ion is produced. The probability of interstitial ion is

$$N_i n = \frac{N_i!}{(N_i - n)! n!}$$

$N_i$  is the number of interstitial positions in crystal.

Notes

The probability of Frankel defect is:

$$W = \frac{N!}{(N-n)! n!} \times \frac{N_i!}{(N_i - n)! n!}$$

3.45 Kb

Birthday / Anniversary



| S  | M  | T  | W  | T  | F  | S  |
|----|----|----|----|----|----|----|
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| 13 | 14 | 15 | 16 | 17 | 18 | 19 |
| 20 | 21 | 22 | 23 | 24 | 25 | 26 |
| 27 | 28 | 29 | 30 | 31 |    |    |

8.00

Acc. to Boltzmann Statistics:

$$S = k_B \log w$$

9.00

So,  $U = nE$  (previously done)

10.00

$$F = U - TS$$

11.00

$$F = nE - k_B T \log \left[ \frac{N!}{(N-n)! n!} \times \frac{N_i!}{(N_i-n)! n!} \right]$$

12.00

$$F = nE - k_B T \log N_i! + \log N! - 2 \log n! - \log [(N-n)!] - \log (N_i-n)! - \log (N_i-n)! - \log (N_i-n)! - \log (N_i-n)!$$

1.00

2.00

Using Stirling approximation  
 $\log x! = x \log x - x$

3.00

$$F = nE - k_B T [N \log N - N + N_i \log N_i - N_i - 2 \log n^n + 2n - (N-n) \log (N-n) + N - n - (N_i-n) \log (N_i-n) + N_i - n]$$

5.00

6.00

$$F = nE - k_B T [N \log N + N_i \log N_i - 2 \log n^n - (N-n) \log (N-n) - (N_i-n) \log (N_i-n)]$$

7.00

8.00

Differentiating w.r.t. n

$$\frac{dF}{dn} = E - k_B T \left[ -2 \log n + \frac{(N-n)}{(N-n)} + \log (N-n) + \frac{(N_i-n)}{(N_i-n)} + \log (N_i-n) \right]$$

Notes

$$\frac{dF}{dn} = E - k_B T \left[ -\log n^2 + \log (N-n) + \log (N_i-n) \right]$$

Birthday / Anniversary



29

Sunday

November 2009

Week 48

Day 333 • 032

Date 29 • 11 • 2009

|        | S  | M  | T  | W  | T  | F  | S  |
|--------|----|----|----|----|----|----|----|
|        | 1  | 2  | 3  | 4  | 5  | 6  | 7  |
| NOV 09 | 8  | 9  | 10 | 11 | 12 | 13 | 14 |
|        | 15 | 16 | 17 | 18 | 19 | 20 | 21 |
|        | 22 | 23 | 24 | 25 | 26 | 27 | 28 |
|        | 29 | 30 |    |    |    |    |    |

Equating  $\frac{df}{dn} = 0$  [For minimum defect]

$$0 = E - k_B T \left[ \log \left( \frac{(N-n)(N_i-n)}{n^2} \right) \right]$$

$$\frac{E}{k_B T} = \log \frac{(N-n)(N_i-n)}{n^2} \quad \left[ \begin{array}{l} N \gg n \\ N_i \gg n \end{array} \right]$$

$$e^{E/k_B T} = \frac{NN_i}{n^2} \quad n^2 = e^{E/k_B T} N \cdot N_i$$

$$n = (NN_i)^{1/2} e^{-E/2k_B T} \quad \left[ n = \sqrt{N \cdot N_i} e^{E/k_B T} \right]$$

Simple Structures :

NaCl Structure :

1). NaCl structure is face centered cubic cell. Each Sodium atom is placed at corners of each unit cell and on faces of each unit cell. Similarly, Chlorine atom is placed at edge centered and body of the unit cell.

2). Each  $\text{Na}^+$  ions are surrounded

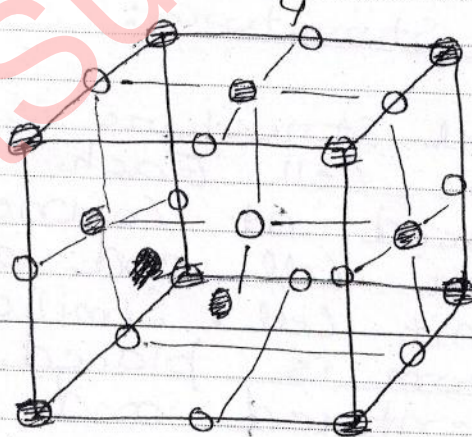
Birthday / Anniversary



by Six  $\text{Cl}^-$  ions and Similarly, each  $\text{Cl}^-$  ion is surrounded by Six  $\text{Na}^+$  ions. Thus, NaCl structure has 6:6 Coordination.

3). The unit cell of NaCl structure has four NaCl unit i.e. 4  $\text{Na}^+$  ions and 4  $\text{Cl}^-$  ions. Since, 8 Sodium atom is present at corner of unit cell and 6 Na atom on faces of unit cell. Thus, Na atom per unit cell 
$$\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$$

Similarly, 12  $\text{Cl}^-$  atoms are placed at edge and 1 at body of unit cell. 
$$1 + 12 \times \frac{1}{4} = 4.$$



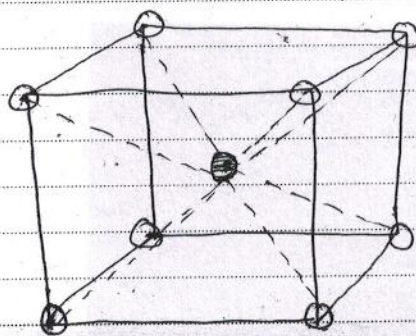
● - Na atom  
○ - Cl atom



## Caesium chloride Structure:

- 1). CsCl Structure is Simple Cubic Crystal. In this Cs atoms are present at corners of each unit cell and Cl atom is placed at body of each unit cell.
- 2). In CsCl Structure,  $\text{Cs}^+$  atoms are shared by eight Cl atoms and  $\text{Cl}^-$  atoms are shared by eight  $\text{Cs}^+$  atoms. Thus, CsCl structure has 8:8 coordination.
- 3). A unit cell of CsCl contains one unit of CsCl i.e. 1  $\text{Cs}^+$  and 1  $\text{Cl}^-$  ion. Thus, atom at corners of the unit cell is not shared by other unit cell.  
For  $\text{Cl}^-$ , = 1

For Cs, 1 (atom at body of unit cell)



○ - Cs atom

● - Cl atom



DECEMBER  
2009

NOVEMBER 2009

| S  | M  | T  | W  | T  | F  | S  |
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JANUARY 2010

| S  | M  | T  | W  | T  | F  | S  |
|----|----|----|----|----|----|----|
| 31 |    |    |    |    | 1  | 2  |
| 3  | 4  | 5  | 6  | 7  | 8  | 9  |
| 10 | 11 | 12 | 13 | 14 | 15 | 16 |
| 17 | 18 | 19 | 20 | 21 | 22 | 23 |
| 24 | 25 | 26 | 27 | 28 | 29 | 30 |

| WK | SUN | MON | TUE | WED | THU | FRI | SAT |
|----|-----|-----|-----|-----|-----|-----|-----|
| 49 |     |     | 1   | 2   | 3   | 4   | 5   |
| 50 | 6   | 7   | 8   | 9   | 10  | 11  | 12  |
| 51 | 13  | 14  | 15  | 16  | 17  | 18  | 19  |
| 52 | 20  | 21  | 22  | 23  | 24  | 25  | 26  |
| 53 | 27  | 28  | 29  | 30  | 31  |     |     |



*Follow complete programme  
conscientiously for a few months,  
and you will develop a new mental  
freshness, giving you the ability to  
make full use of your powers.*

DEC