

THEORY & OBJECTIVE

MATERIAL SCIENCE

*By
Team of
Engineers Academy*



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BASICS OF ENGINEERING MATERIAL

THEORY

1.1 | CHEMICAL BONDS

The binding force between two or more atoms or molecules are known as chemical bonds.

There are two types of chemical bonds.

- Primary
- Secondary

1.1.1 Primary Bond

These bond are inter atomic bond.

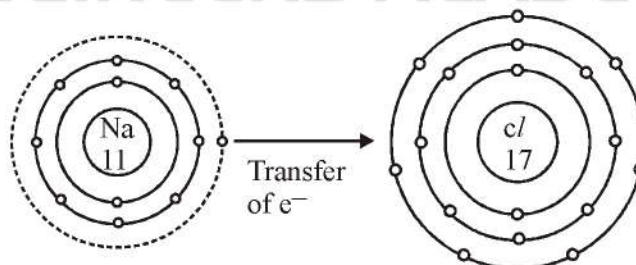
These bond are having higher bond energy.

Ex. Ionic, covalent and metallic bond.

Ionic Bond : Ionic bond is a bond resulting from the electrostatic interaction of opposite ions by transfer of e^- from one to another.

Ionic solid are formed particularly elements on the left and right hand side of the periodic table.

Ex. Alkali halide (Group I and Group VII elements) $NaCl$, KCl et.)

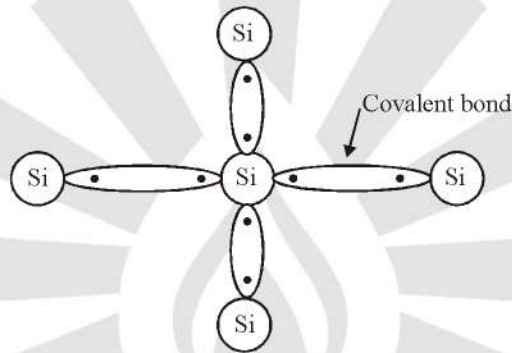


General Characteristic of Ionic Bond

- Moderate to high strength
- Higher hardness
- Brittle (can be break)
- Malleable (can be mould)
- Electrically neutral
- High melting point

Covalent Bond : Covalent bond is formed by sharing of e^- between neighboring atoms.

Ex. Si, Ge, CO_2 .

**General Characteristic of Covalent Bond**

- High strength
- High melting point
- Brittle
- Electrical conductivity depends upon Bond strength
- Tin : Conductor (weak covalent bond)
- Si, Ge : Semi conductor (moderate)
- Diamond : Insulator (High)

Metallic Bond : This type of bond is in the element having small number of valence electron, which are loosely held, so that they can be easily released to the common pool.

The Metallic bonding results when each of the atoms of the metal contributes its valence e^- to the formation of an e^- cloud that pervades the solid metal.

General Characteristic of Metallic Bond

- High electrical and thermal conductivity
- Metals are opaque

- They are having surface luster
- Metallic bond are non directional (it means bond strength is equal in all direction)

Ex. Alkali metals (highest metallic bonding)

1.1.2 Secondary Bond

These bonds are inter molecular bond.

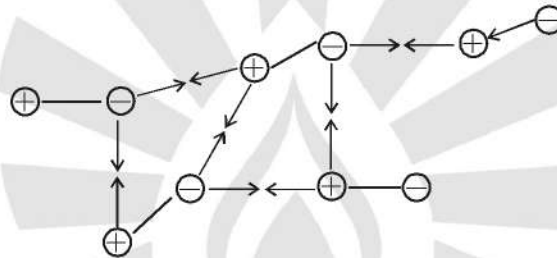
These bonds are having lesser bond energy as compare to primary bond.

Ex. Vanderwall bond, hydrogen bond.

Vanderwall Bond : Weak or secondary bond known as vander wall force can link molecules that posses a non symmetric distribution of charge.

Dipole interaction between molecules or atoms is due to presence of vanderwall force of attraction.

Ex. HF, H₂O, solid Ar, Solid He, solid hydrogen etc.



Hydrogen bond is a strong type of vanderwall's bond

1.2 | ATOM ARRANGEMENT IN MATERIALS

Arrangement of atoms in a material has significant effect on properties.

Depending on the manner of atomic grouping, materials are classified as

1.2.1 Molecular Structure

Molecular structure have a distinct number of atoms that are held together by primary bonds, but they have only relatively weak bonds with other similar group of atoms.

Ex. O₂, H₂O, C₂H₄ etc.

1.2.2 Crystal Structure

Crystal structure are assumed by solid materials and most minerals.

Atoms are arranged in a regular geometrical array known as space lattice.

1.2.3 Amorphous Structure

The atoms have a certain degree of local order but when viewed as an aggregate, have a more disorganized atoms arranged than the crystalline solid.

Ex. Glass

1.3 | ATOMS ARRANGEMENT IN SOLID**1.3.1 Crystalline Material**

Atoms self-organize in a periodic manner is called crystalline material.

1.3.2 Single Crystal Material

Atoms are in a repeating or periodic manner over the entire extent of the material.

These material are anisotropic materials.

Ex. Quartz.

Anisotropic Material : The material in which properties depend on the direction in which they are measured is called anisotropic material.

Ex. Single crystal material

Isotropic Material : The material in which properties are independent of the direction in which they are measured is called isotropic material.

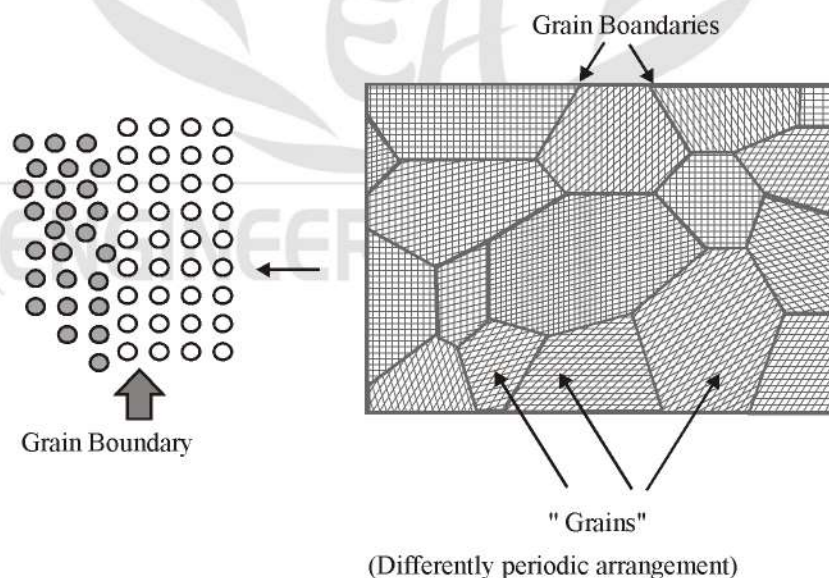
Ex. Polycrystalline material

1.3.3 Poly Crystalline Material

These material are divided into no. of small regions. These regions are called grain. within each grain. molecular arrangement is regular or periodic but this arrangement varies from are grain to another.

Ex. Polycrystalline silicon

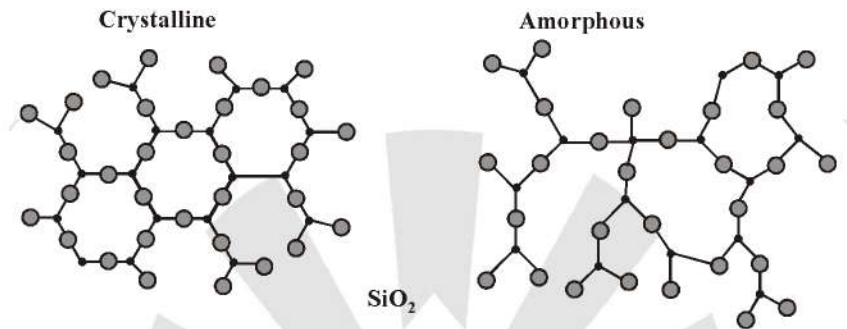
These materials are isotropic



1.3.4 Amorphous Material

In amorphous material, atoms upto first nearest neighbour are arranged periodically but atoms which are far away from nearest atoms are found to be arranged randomly.

When atoms or molecules are not given opportunity to arrange in periodic or regular manner, an amorphous materials may be formed.



Ex. Super cooled state of SiO_2 is called glass (amorphous material)

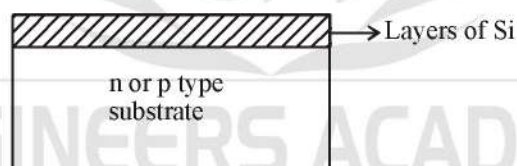
Note :

- On annealing (heating and cooling) SiO_2 crystallizes into Quartz.
- In some cases molecules may be extremely long and irregular in shape so that periodic or regular arrangement may not be obtained.

Ex. Polymers

1.3.5 Epitaxial Material

The process of growth of a layer of silicon over a substrate is called epitaxial and the material through layer is made is called epitaxial material.



1.4 | UNIT CELL

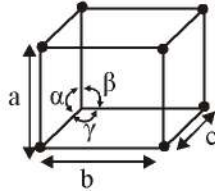
It is defined as the minimum area cell in 2-dimension or minimum volume cell in 3 dimension by repetition of which a crystal may be formed.

Parameters of unit cell :

- Unit cell dimension
- Angle between axis

- Number of atoms per unit cell
- Co-ordination number
- Atomic packing factor (APF)

Ex. $\angle \alpha : a, c$
 $\angle \beta : b, a$
 $\angle \gamma : c, b$



Co-ordination Number : The no. of atoms which are in physical contact with a particular atoms in a crystal structure is called co-ordination number.

Atomic packing factor (APF) : APF or packing efficiency indicates how closely atoms are packed in unit cell.

$$APF = \frac{\text{No. of atoms per unit cell} \times \text{Atomic volume}}{\text{Volume of unit cell.}}$$

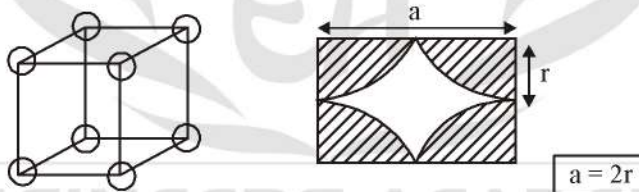
Lattice : Periodically or orderly arrangement of unit cell is called lattice.

1.5 | CUBIC CRYSTAL STRUCTURE

1.5.1 Simple Cubic

In a simple cubic there are 8 atoms at eight corner of a cube.

Atoms are in physical contact along edge of the cube.



$$\text{No. of atoms per unit cell} = 8 \times \frac{1}{8} = 1$$

$$APF = \frac{1 \times \frac{4}{3} \pi r^3}{a^3} = \frac{\frac{4}{3} \pi \left(\frac{a}{2}\right)^3}{a^3} = 0.52$$

Co-ordination no. = 6.

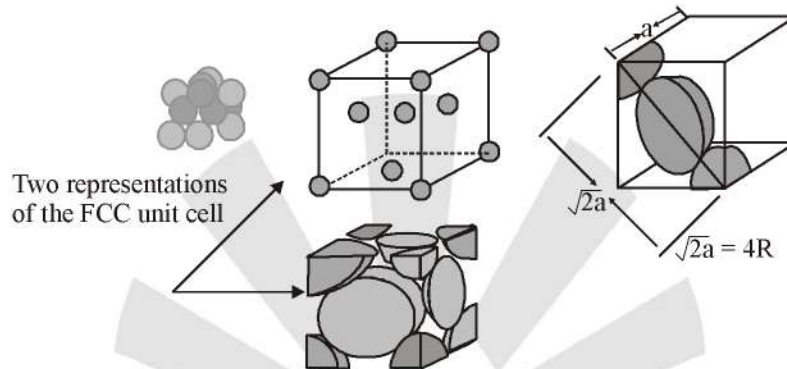
Ex. Mn, Polonium, Flourspar etc

1.5.2 Face Centered Cubic (FCC)

In FCC, there are 8 atoms at 8 corner of the cube and 6 atom at the centre of 6 faces of the cube.

$$\text{No. of atoms per unit cell} = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$$

Atoms are in physical contact along face diagonal



Cube length edge

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

$$\text{APF} = \frac{4 \times \frac{4}{3} \pi r^3}{a^3} = 0.74.$$

Co-ordination number = 12

Corner and face atoms in the unit cell are equivalent

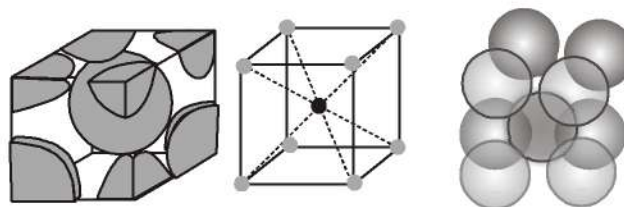
FCC crystal structure has APF of 0.74, the maximum packing for a system (FCC has closed pack structure).

Ex. Gold (Au), Ag, Pt, Cu, Ni, Pb, Fe (γ -type), Al etc.

1.5.3 Body Centered Cubic (BCC)

In BCC, 8 atoms are at 8 corners of cube and one atoms is located at the center of unit cell.

Atoms are in physical contact along body diagonal or in cubic diagonal.

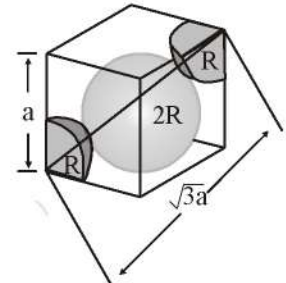


Cube edge length, $a = \frac{4R}{\sqrt{3}}$

Co-ordination number = 8

No. of atoms per unit cell = $8 \times \frac{1}{8} + 1 = 2$

$$APF = \frac{2 \times \frac{4}{3} \pi R^3}{a^3} = 0.68$$



Body and corner atoms of unit cell are equivalent

Ex. Li, Na, K, Cr, Mn, Cb, W, Ti, Fe (α - iron, δ -iron) etc.

1.5.4 Diamond Cubic

Diamond cubic unit cell is having contribution of 18 atoms, out of 18 atoms

- (i) 8 atoms are corner atoms
- (ii) 6 atoms are face centered atoms
- (iii) Remaining 4 atoms are completely inside

No. of atoms per unit cell = $8 \times \frac{1}{8} + 6 \times \frac{1}{2} + 4 = 8$

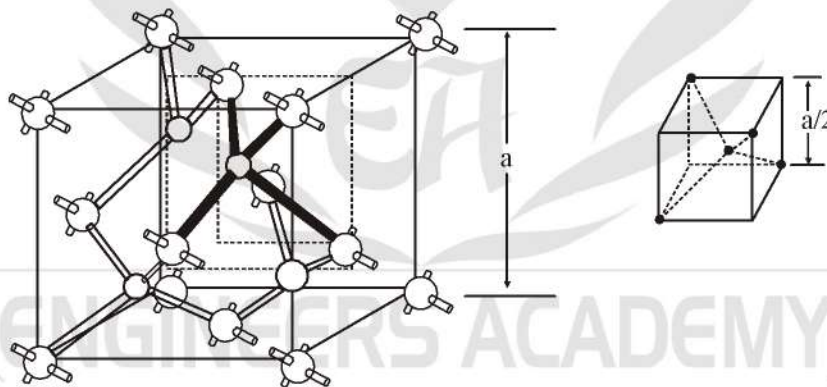


Fig. : Tetrahedral Structure of Closest Neighbor in Diamond Lattice

Length of cube $a = 8r/\sqrt{3}$ or $r = a \sqrt{3}/8$

$$APF = \frac{8 \times \frac{4}{3} \pi r^3}{a^3} = 0.34$$

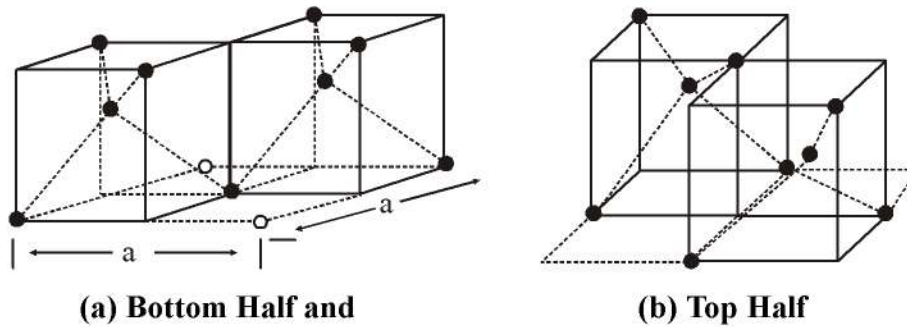


Fig. : Portions of the Diamond Lattice

Diamond cubic structure is similar to zinc blende structure

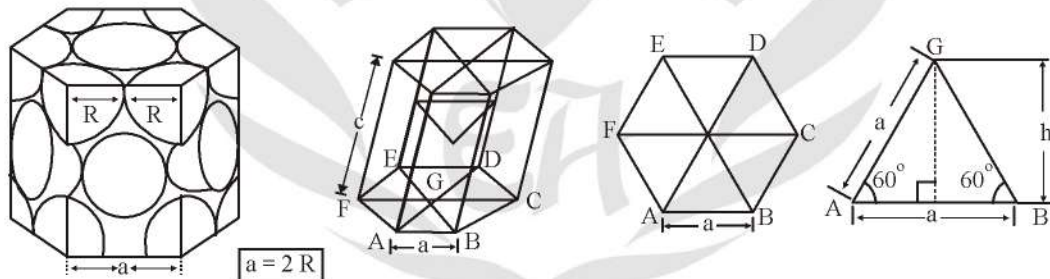
Group (III-V) compounds are having zinc blende structure

Ex. Diamond, C, Si, Ge, group II-V compounds

1.5.5 Hexagonal Close Packing (HCP)

HCP unit cell is having

- (i) 12 corner atoms
- (ii) 2 face centre atoms in top and bottom hexagon
- (iii) 3 atoms are inside

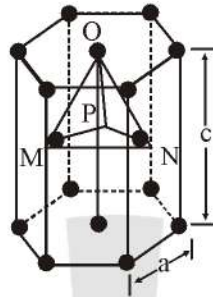


$$\text{No. of atoms per unit cell} = 3 + 2 \times \frac{1}{2} + \frac{1}{6} \times 12 = 6$$

$$\frac{c}{a} = \frac{\text{max}^m \text{ dimension}}{\text{min}^m \text{ dimension}} = 1.63$$

$$\begin{aligned} \text{Unit Cell Volume} &= \left(6 \times \frac{1}{2} \times a \times h \right) \times c \\ &= (3 \times a \times a \sin 60^\circ) \times c \\ &= 3a^2 c \sin 60^\circ \end{aligned}$$

The face-centered atom and the three mid-layer atoms from a tetrahedron MNOP which has sides equal to a (as atoms at vertices touch each other) and height of $c/2$. Using this tetrahedron it can be shown that for an ideal hexagonal crystal c/a ratio = 1.633.



$$APF = \frac{6 \times \frac{4}{3} \pi R^3}{3a^2 c \sin 60^\circ} = \frac{8\pi a^3}{3 \times 8 \times 1.414 a^3} = 0.74$$

Co-ordination number of HCP unit cell is 12.

Ex. Be, Cd, Mg, Zn, Zr, etc.

Note :

- HCP and FCC are also called closed pack structure as their packing efficiency is highest i.e., 74%

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OBJECTIVE SHEET

1. In a Si crystal, the arrangement of atoms repeats periodically, this type of material is classified as
 - (a) Amorphous and non crystalline
 - (b) Non crystalline and epitaxial
 - (c) Amorphous and single crystal
 - (d) Epitaxial and single crystal
2. When BCC iron is heated, it changes to FCC iron resulting
 - (a) Increase in volume
 - (b) Contraction in volume
 - (c) No Change in volume
 - (d) Crack in the in material
3. Consider statements related to FCC structure
 1. Co-ordination number is 12
 2. APF is 0.74
 3. There is an atom at the body center of the unit cell.

Which of the following statement are correct

 - (a) 1 and 2
 - (b) 2 and 3
 - (c) 1 and 3
 - (d) 1, 2, 3
4. Consider statement related diamond structure
 1. Co-ordination number is 4
 2. Packing efficiency is 34%
 3. Crystallizes into diamond structure

Which of the following statement are correct

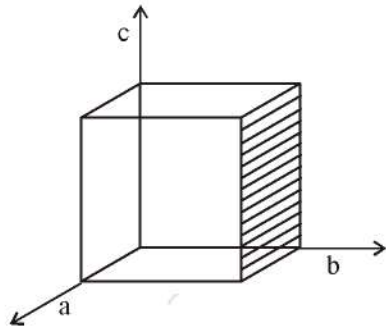
 - (a) 1 and 2
 - (b) 2 and 3
 - (c) 3 and 1
 - (d) 1, 2, 3
5. **Assertion (A)** : Atomic number of sodium is 11
Reason (R) : Sodium has a body centred cubic lattice
 - (a) Both A and R are true and R is the correct explanation of A
 - (b) Both A and R are true, but R is not the correct explanation of A
 - (c) A is true, but R is false
 - (d) R is true, but A is false
6. A material has FCC structure with atomic radius 1.06\AA . calculate interplanar separation for $\{1, 1, 0\}$ planes.
 - (a) 3.12\AA
 - (b) 1.12\AA
 - (c) 2.12\AA
 - (d) 4.13\AA
7. For Rhombohedral structure, the lattice parameters are
 - (a) $a = b = c, \alpha = \beta = \gamma \neq 90^\circ$
 - (b) $a = b = c, \alpha = \beta = 90^\circ; \gamma \neq 90^\circ$
 - (c) $a = b \neq c, \alpha = \beta = 90^\circ; \gamma = 120^\circ$
 - (d) $a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$
8. Read the following statements with respect to Single crystalline materials
 1. Periodic and repeated arrangement of atoms is perfect
 2. They are not existed naturally, they produced only artificially
 3. Electronic micro circuit is made up of single crystalline material

Of the above the correct statements are:

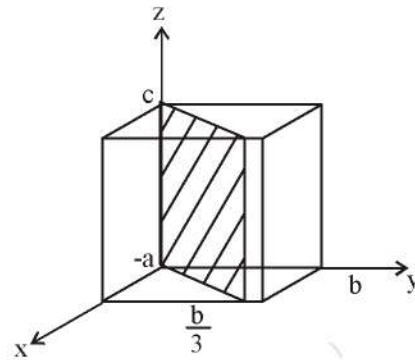
 - (a) 1, 2
 - (b) 1, 2 & 3
 - (c) 1, 3
 - (d) 2, 3
9. Which of the following statements is/are true for the diamond structure?
 1. Coordination number is four.
 2. Packing fractions is 0.34
 3. Copper crystallizes into diamond structure
 4. Lattice is FCC.
 - (a) 1 only
 - (b) 1, 2 and 4
 - (c) 2 and 3
 - (d) 2, 3 and 4

20. Calculate Miller indices

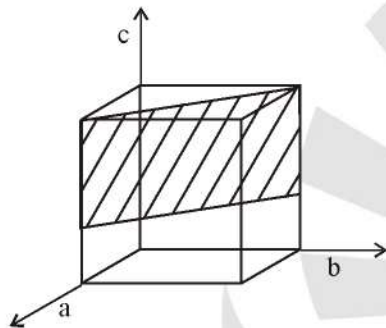
(i)



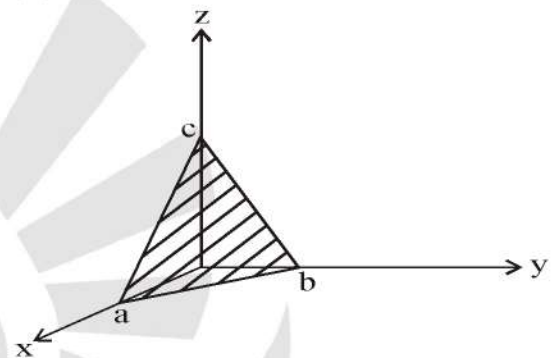
(iii)



(ii)



(iv)



□□□

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ANSWER SHEET

1. *Ans. (d)*
 2. *Ans.*
 BCC iron

$$a\sqrt{3} = 4r$$

$$r = \frac{a\sqrt{3}}{4}$$

FCC iron

$$a\sqrt{2} = 4r ; a = 2\sqrt{2}r ; r = \frac{a}{2\sqrt{2}}$$

Therefore there is contraction in volume.

3. *Ans. (a)*
 4. *Ans. (d)*
 5. *Ans. (b)*
 6. *Ans. (c)*

Given data

$$r = 1.06 \text{ \AA}$$

$$[l, m, n] = [1, 1, 0]$$

For FCC : $a\sqrt{2} = 4R$

$$a = 2\sqrt{2}r$$

$$d = \frac{a}{\sqrt{l^2 + m^2 + n^2}}$$

$$= 2r = 2 \times 1.06 \text{ \AA}$$

$$= 2.12 \text{ \AA}$$

7. *Ans. (a)*
 8. *Ans. (c)*
 9. *Ans. (b)*
 10. *Ans. (a)*
 11. *Ans. (d)*
 12. *Ans. (d)*

13. *Ans. (a)*
 14. *Ans. (a)*
 15. *Ans. (c)*
 16. *Ans. (a)*
 17. *Ans. (d)*
 18. *Ans. (a)*

Ionic crystals are hard and brittle.

19. *Ans. (b)*

20.(i) *Ans.*

- $\infty, b, \infty,$
 $\infty, 1, \infty,$
 $0, 1, 0,$
 $[0, 1, 0,]$

(ii) *Ans.*

- $a, b, \infty,$
 $1, 1, \infty,$
 $1, 1, 0,$
 $[1, 1, 0,]$

(iii) *Ans.*

- $-a, \frac{b}{3}, \infty$
 $-1, \frac{1}{3}, \infty$
 $1, 3, 0$
 $[-1, 3, 0]$

(iv) *Ans.*

- $a, b, c,$
 $1, 1, 1,$
 $1, 1, 1,$
 $[1, 1, 1,]$

