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PH8151 ENGINEERING PHYSICS

UNIT-V CRYSTAL PHYSICS

13-Marks

1. a) Derive an expression for the inter-planar distance a simple cubic crystal

[OR]

b) Derive the relation between inter-planar distance (d) and lattice constant (a) of a cubic crystal.

The inter-planar distance is the perpendicular distance between successive parallel planes of atoms in a crystal.



Consider a cubic crystal with 'a' as the cube edge. Let ABC be a plane in the cubic crystal. Let (h K I) be the miller indices for the plane ABC. Imagine another parallel plane passing through the origin. Let ON = d be the inter-planar distance. Then the intercepts of the plane on three axes are

$$OA : OB : OC := \frac{a}{h} : \frac{a}{k} : \frac{a}{l}$$

$$OA = \frac{a}{h}, OB = \frac{a}{k}, OC = \frac{a}{l}$$
From NOA, $\cos \alpha = \frac{OA}{OB} = \frac{d}{\frac{a}{h}} = \frac{dh}{a}$
From NOB, $\cos \beta = \frac{OA}{OB} = \frac{d}{\frac{a}{k}} = \frac{dk}{a}$
From NOC, $\cos \gamma = \frac{OA}{OC} = \frac{d}{\frac{a}{l}} = \frac{dl}{a}$
From the law of direction of cosines, $\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma$

$$\left(\frac{dh}{a}\right)^2 + \left(\frac{dk}{a}\right)^2 + \left(\frac{dl}{a}\right)^2 = 1$$

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$$\left(\frac{d}{a}\right)^2 (h^2 + k^2 + l^2) = 1$$
$$d^2 = \frac{a^2}{h^2 + k^2 + l^2}$$
$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

This is the relation between interplanar spacing (d), cube edge (a) and Miller indices (h k l).

2. What are line defects? Explain edge dislocation and screw dislocation.

The defects, which take place due to distortion or dislocation of atoms along a line in some direction, are called line defects.

Line defects are also called dislocations or one-dimensional defects.

The two basic types of dislocation are

(a) Edge dislocation

(b) Screw dislocation

Edge dislocation:

Whenever a half plane of atoms is inserted between the planes of atoms in a perfect crystal, the defect is known as edge dislocation.



If the extra half plane of inserted atoms lies above the slip plane, the line defect is called positive dislocation and is denoted by the symbol perpendicular. If the extra half plane lies below the slip plane, the defect is called negative dislocation and is denoted by the symbol T. The horizontal line in the symbol represents the slip plane or line of dislocation and the vertical line represent the incomplete atomic plane.

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Screw dislocation:

Whenever the atoms are displaced in two separate planes perpendicular to each other, the defect produced is called screw dislocation. Screw dislocation is due to the displacement of atoms in one part of the crystal related to the other part of the crystal forming a spiral ramp around the dislocation line. It is also known as Burger's dislocation.

A screw dislocation may be understood by slip process as shown in figure.



Let a sharp cut ABCD be made partway through a perfect crystal. Let the crystal on one side of the cut be displaced relative to the other side parallel to the curve, shaded area ABB' indicates region of slip-plane. The dislocation is represented by line AD.

3. (a) Write a note on point imperfections in crystals.

[OR]

b) Write short notes on crystal imperfections and its advantages.

The defects, which take place due to imperfect packing of atoms during crystallization, are known as point defects. They are also called zero dimensional imperfections. The common point defects are

- (a) Vacancies
- (b) Interstitials
- (c) Impurities
- (d) Electronic defects

(a) Vacancies:

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A vacancy refers to the unoccupied position of an atom or vacant site within the crystal lattice.



Such defect is caused due to the imperfect alignment of atoms during the crystalline process or from thermal vibration of atoms at high temperatures. Vacancies may be single or two or more of them may condense into a divacancy or tri-vacancy.

Schottky defect:

When a pair of positive and negative ions is missing from an ionic crystal, the defect caused is known as Schottky defect. Since a pair is missing, electrical neutrality is maintained.



(b) Interstitials:

Whenever an exam atom occupies interstitial position (voids), without disturbing the parent atom in the crystal system, the defect caused is known as interstitial defects.

The interstitial atom may be either a normal atom from the same crystal or an impure atom which is not present in the lattice.

An atom can enter the interstitial space or void only if it is smaller than the parent atom otherwise, it will cause atomic distortion or strain because the interstitial atom tends to push the surrounding atoms further apart.

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By giving enormous stress, some of the parent atoms move from their lattice sites and occupy the interstitials present in the crystal. This type of imperfections is called self-interstitial imperfections.

Frenkel defect:



(c) Impurities:

Impurity defects are foreign atoms introduced into a crystal lattice. There are two types of impurities.

- (i) Substitutional impurity
- (ii) Interstitial impurity

A substitutional impurity is created when a foreign atom replaces a parent atom in the lattice.



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An interstitial impurity is created when a small atom occupies the interstitial space of the crystal lattice. These defects are responsible for the functioning of most semiconductor devices.



(d) Electronic defects:

Electronic defects are the result of errors in charge distribution in solids. These defects are free to move in the crystal under the influence of an electrical field. This accounts for some electronic conductivity of certain solids.

4. a) Show by a neat diagram the HCP structure. Show by a neat diagram the HCP structure and the ratio $c/a = \sqrt{8/3}$

[OR]

b) Define packing factor. Describe the HCP structure. Show that for an HCP structure $c/a = \sqrt{8/3}$ and hence calculate the packing factor for the HCP structure.

<u>i) HCP</u>



ii) In a hexagon a closed packed structure the unit cell has one atom at each of the 12 corners of the hexagonal prism, one atom at the centre of the two

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hexagonal faces and 3 atoms symmetrically arranged in the body of the cell at a distance c/2 from the bottom layer.



Image source: www.vedantu.com

i) Number of atoms per unit cell:

Each corner atom is shared by six-unit cells.

Number of atoms in the upper hexagonal plane of the unit cell = $1/6 \times 6 = 1$ atom.

Number of atoms in the lower hexagonal plane = $1/6 \ge 6 = 1$ atom

Each central atom is shared by two-unit cell

Number of atoms contributed by both atoms in upper and lower planes = 1/2 x2=1 atom

Centre body atoms = 3 atoms

The number of atoms per unit cell = 2+1+3=6 atoms

ii) Coordination number:

The central atom has 6 nearest neighboring atoms in the same plane. There are two layers one above and the other below the bottom layer containing 3 atoms in each layer.

Coordination number is 12.

iii) atomic radius:

The atoms touch each other along the edge of the hexagon. The nearest neighboring distance is 2r.

a = 2r, r = a/2

iv) Calculation of c/a ratio:

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"C" is the height of the unit cell and 'a' is the distance between the two neighboring atoms. The three body atoms lie in a horizontal plane at height c/2 from the bottom.

Consider the $\triangle ABO$ in the bottom layer of the HCP structure.



 $In \ \Delta ABY, < YAB = 30^{\circ}, \quad \cos 30^{\circ} = AY/AB, \quad AY = AB \cos 30^{\circ} = a\sqrt{3/2}$ ------ (1)

But AX = 2/3 AY, $2/3 x a\sqrt{3/2}$, $AX = a/\sqrt{3}$ ------(2)

In $\triangle AXD$ $AD^2 = AX^2 + DX^2$ $a^2 = (a/\sqrt{3})^2 + (c/2)^2, a^2 = a^2/3 + c^2/4, c^2/4 = a^2 - a^2/3$ $c^2/4 = 2a^2/3, c^2/a^2 = 4 \times 2/3 = 8/3$ $c/a = \sqrt{8/3} = 1.666$ ------(3)

 $Packing \ Factor = \frac{Volume \ occupied \ by \ the \ atoms \ in \ an \ unit \ cell(v)}{Volume \ of \ the \ unit \ cell(v)}$

Volume occupied by the atoms in a unit cell (v) = No. of atoms per unit cell x Volume of 1 atom

$$v = 6 \ x \ \frac{4}{3}\pi r^3, \ v = 6 \ x \ \frac{4}{3}\pi \left(\frac{a}{2}\right)^3$$

 $v = \pi a^3$

Volume of the unit cell (v) = Area of Hexagon x Height of the unit cell Volume of the unit cell (v) = 6 x Area of $\triangle ABO \ x$ Height of the unit cell Volume of the unit cell (v) = 6 x $\frac{1}{2}$ x AY x BO x Height of the unit cell Volume of the unit cell (v) = 6 x $\frac{1}{2}$ x $\frac{a\sqrt{3}}{2}$ x a x c Volume of the unit cell (v) = $\frac{3\sqrt{3}a^2c}{2}$

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Packing Factor $=\frac{\pi a^3}{\frac{3\sqrt{3}a^2c}{2}} = \frac{2\pi}{3\sqrt{3}} \left(\frac{a}{c}\right) = \frac{2\pi}{3\sqrt{3}} x \sqrt{\frac{3}{8}} = \frac{\pi}{3\sqrt{2}} = 0.74$

Packing factor = 74%

5. what is packing factor? Obtain packing factors for SC, BCC, FCC and HCP structures.

i) atomic packing factor is defined as the ratio of the volume occupied by the atoms in a unit. Cell to the volume of the unit cell.

 $Packing \ factor = \frac{Volume \ occupied \ by \ the \ atoms \ in \ an \ unit \ cell}{Volume \ of \ the \ unit \ cell}$

Packing factor of SC structure:

In simple cubic structure, there is one atom at each of the eight corners of the unit cell. These atoms touch along cube edges. ------ (1)

Number of atoms-per unit cell:

There are eight atoms one at each corner of the unit cell. Each corner atom is shared by eight surrounding unit cells. $1/8 \times 8 = 1$ atom

The no of atoms per unit cell is 1 atom

ii) Coordination number:

There are six nearest neighbor atoms. Hence the coordination number

is 6.

iii) Atomic radius:

2r = a

r = a/2 ----- (1)

iv) Packing factor:

 $Packing \ factor = \frac{Volume \ occupied \ by \ the \ atoms \ in \ the \ unit \ cell}{Volume \ of \ the \ unit \ cell}$

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 $=\frac{\frac{4}{3}\pi r^3}{a^3}$

Sub r = a/2, P.F. = $4/3\pi a^3/3 \ x \ 8 \ x \ a^3 = \pi/6 = 0.52$ -----(1)

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

Packing factor of BCC structure:

In Body cantered cubic structure, there are eight corner atoms at the eight corner of the unit cell and one atom at the body centre.

1)Number of atoms per unit cell

Each corner atoms are share by eight-unit cells = $1/8 \times 8 = 1$

Body cantered atom = 1

Total number of atoms per unit cell = 1 + 1 = 2 atoms/unit cell

touches the body centered atom along the body diagonal.

Coordination number = 8



3)Atomic Radius: In BCC structure, the corner atoms do not touch each other. But each corner atom



From figure

 $AD^2 = AC^2 + CD^2$

 $[but AC^2 = AB^2 + BC^2]$

We can write, $AD^2 = AB^2 + BC^2 + CD^2$, $AD^2 = a^2 + a^2 + a^2$

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 $AD^2 = 3a^2$, $AD = a\sqrt{3}$,

Here AD = 4r,

 $4r = a\sqrt{3}$

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

4)Atomic packing factor:

 $Atomic \ factor = \frac{Number \ of \ atoms \ per \ unit \ cell \ x \ Volume \ of \ one \ atom}{Total \ volume \ of \ the \ unit \ cell}$

In BCC,

Number of atoms per unit cell = 2

Volume of 2 atoms = 2 $x \frac{4}{2}\pi r^3$

Radius of atom in BCC $r = a\sqrt{3}/4$

Packing factor = 2 x $4/3\pi r^3/a^3 = \sqrt{3}\pi/8 = 0.68$

Packing factor = 68%

Hence 68% of the volume of unit cell is occupied by atoms and the remaining 32% is vacant.

ii) Face centered cubic structure (FCC)

In a face centered cubic structure, there are eight corner atoms and six face centered atoms at the centre of six faces.



i) Number of atoms per unit cell:

Each corner atom is shared by eight surrounding unit cells. Each face centered is shared by two adjoining unit cells.

Corner atom = $1/8 \times 8 = 1$

Face centered atom = $1/2 \times 6 = 3$

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Total number of atoms = 4 atom / unit cell ------ (1)

ii) Coordination number:

The centre atom touches the four corner atoms and the four face centered atoms on either side parallel to its plane.

The coordination number is 12. ----- (1)

iii) Atomic radius:



The atom in it touches along the diagonal of the face of the cube.

The face diagonal, AC = 4rConsider $\triangle ACB$, $AC^2 = AB^2 + BC^2$ $(4r)^2 = a^2 + a^2$, $16r^2 = 2a^2$

Taking square root we get, $4r = \sqrt{2}a$

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

Hence the lattice constant $a = 4r/\sqrt{2}$ ------ (1)

a. Packing factor:

 $P.F = \frac{Number of atoms/unit cell x volume of one atom}{Volume of the unit cell}$

Number of atoms per unit cell = 4

$$P.F = \frac{4 x \frac{4}{3} \pi r^3}{a^3}$$

Substituting the value of $r = \sqrt{2} a/4$

$$P.F = \frac{4 \ x \ 4 \ x \ \pi \ x \ \sqrt{2} \ x \ \sqrt{2} \ x \ \sqrt{2} \ x \ a^3}{3 \ x \ a^3 \ x \ 4 \ x \ 4 \ x \ 4} = \frac{\pi \sqrt{2}}{6}$$
$$= \pi / 3\sqrt{2} = 0.74 = 74\% \quad -----(2)$$

Hence 74% of the volume of the unit cell is occupied by atoms and the remaining 26% is vacant. Metals like copper, Aluminum, lead, gold and silver have this structure.

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(iii) HCP



Image source: www.vedantu.com

In a hexagon a closed packed structure the unit cell has one atom at each of the 12 corners of the hexagonal prism, one atom at the centre of the two hexagonal faces and 3 atoms symmetrically arranged in the body of the cell at a distance c/2 from the bottom layer.

(i) Number of atoms per unit cell:

Each corner atom is shared by six-unit cells.

Number of atoms in the upper hexagonal plane of the unit cell = $1/6 \times 6 = 1$ atom

Number of atoms in the lower hexagonal plane = $1/6 \times 6 = 1$ atom

Each central atom is shared by two-unit cell

Number of atoms contributed by both atoms in upper and lower planes = $1/2x^2=1$ atom

Centre body atoms = 3 atoms

The number of atoms per unit cell = 2 + 1 + 3 = 6 atoms

(ii) Coordination number:

The central atom has 6 nearest neighboring atoms in the same plane. There are two layers one above and the other below the bottom layer containing 3 atoms in each layer.

Coordination number is 12.

(iii) Atomic radius:

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The atoms touch each other along the edge of the hexagon. The nearest neighboring distance is 2r.

a = 2r, r = a/2

(iv) Calculation of c/a ratio:

"C" is the height of the unit cell and 'a' is the distance between the two neighboring atoms. The three body atoms lie in a horizontal plane at height c/2 from the bottom.

Consider the $\triangle ABO$ in the bottom layer of the HCP structure



Volume occupied by the atoms in a unit cell (v) = No. of atoms per unit cell x Volume of 1 atom

$$v = 6 x \frac{4}{3}\pi r^3$$
$$v = 6 x \frac{4}{3}\pi \left(\frac{a}{2}\right)^2$$

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 $v = \pi a^3$

Volume of the unit cell (v) = Area of Hexagon x Height of the unit cell

Volume of the unit cell (v) = 6 x Area of $\triangle ABO$ x Height of the unit cell

Volume of the unit cell (v) = $6 \times \frac{1}{2} \times AY \times BO \times Height of the unit cell$

Volume of the unit cell $(v) = 6 x \frac{1}{2} x \frac{a\sqrt{3}}{2} x a x c$

Volume of the unit cell $(v) = \frac{3\sqrt{3}a^2c}{2}$

Packing Factor
$$=$$
 $\frac{\pi a^3}{\frac{3\sqrt{3}a^2c}{2}} = \frac{2\pi}{3\sqrt{3}} \left(\frac{a}{c}\right)$

$$=\frac{2\pi}{3\sqrt{3}} x \sqrt{\frac{3}{8}} = \frac{\pi}{3\sqrt{2}} = 0.74$$

Packing factor = 74%

6. i) Explain various crystal systems with neat diagrams.

ii) Describe the steps to determine Miller indices and also mention its importance.

 a) i) The seven crystal system can be arranged in fourteen possible types of space lattices.

The 14 lattices are called Bravais lattices.

b) Cubic system: $(a = b = c \text{ and } \alpha = \beta = \gamma = 90^{\circ})$

Cubic lattice has three possible types of lattices-simple cubic, body centered cubic and Face centered cubic lattices.

System		
Cubic	$a = b = c$, $\alpha = \beta = \gamma = 90^{\circ}$	
Tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90^{\circ}$	
Orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90^{\circ}$	is is is
Rhombohedra	$a = b = c, \alpha = \beta = \gamma \neq 90^{\circ}$	A B B B B B B B B B B B B B B B B B B B

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Hexagonal	$a = b \neq c, \alpha = \beta = 90^{\circ}, \gamma$ = 120°	
Monoclinic	$a \neq b \neq c, \alpha = \gamma = 90^{\circ} \neq \beta$	
Triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^{\circ}$	e b b
		q q

Tetragonal system: $a = b \neq c$ and $\alpha = \beta = \gamma = 90^{\circ}$

Tetragonal lattice has two possible types of lattices-simple tetragonal body centered. Orthorhombic lattice has four possible types of lattices-simple orthorhombic, body

centered orthorhombic, Face centered orthorhombic and base centered orthorhombic lattices.

Monoclinic system: $a \neq b \neq c$ and $\alpha = \beta = 90^{\circ}, \gamma \neq 90^{\circ}$

Monoclinic lattice has two possible types of lattices-simple monoclinic, base centered monoclinic.

Triclinic system: $a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma \neq 90^{\circ}$

Triclinic lattice has only one possible type of lattice-simple trigonal.

Trigonal or Rhombohedral system: a = b = c and $(\alpha = \beta = \gamma) \neq 90^{\circ}$

Trigonal lattice has only one possible type of lattice-simple trigonal.

Hexagonal system: $a = b \neq c$ and $\alpha = \beta = 90^{\circ} \gamma = 120^{\circ}$

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Hexagonal lattice has only one possible type of lattice-simple hexagonal.

The following table. Shows the seven crystal system which are divided into 14 Bravais lattices along with the unit cell parameters and examples.

	S.no	Crystal systems	Unit cell parameters	Examples	Bravais lattices	Number of lattices in the system
	1.	Cubic	a = b = c $\alpha = \beta = \gamma$ $= 90^{\circ}$	NaCI, CaF _{2,} NaCIO ₃	Simple Body centered Face centered	3
	2.	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma$ $= 90^{\circ}$	NiSO4, SnO2, Indium	Simple Body centered	2
	3.	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma$ $= 90^{\circ}$	MgSO ₄ , KNO ₃ , Topaz	Simple Base centered Body centered	4
					Face Centered	
	4.	Monoclinic	$a \neq b \neq c$ $\alpha = \beta$ $= 90^{\circ}$ $\gamma \neq 90^{\circ}$	NaSO4, FeSO4	Simple Base centered	2
	5.	Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$ $\neq 90^{\circ}$	CuSO4, K2Cr2O7	Simple	1
	6.	Trigonal or Rhombohedral	a = b = c ($\alpha = \beta$ = γ) \neq 90°	CaSO4, Sb, Calcite	Simple	1
	7.	Hexagonal	$a = b \neq c$ $\alpha = \beta$ $= 90^{\circ}$ $\gamma = 120^{\circ}$	Tourmaline, Quartz, Zn, Mg	Simple	1

ii) Miller indices:

Miller introduced a system with a set of three numbers within brackets to design a plane in a crystal.

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The set of three numbers within brackets obtained from the reciprocals of the intercepts made by the planes on the crystallographic axes is called Miller indices.

Explanation:

Let us consider a plan ABC that cut 1 unit along the X-axis, 3 units along Y-axis and 2 units along Z-axis as shown in the fig.



Image source: www.spiedigitallibrary.org

Here intercepts values are (1, 3, 2)

The reciprocals are 1, 1/3, 1/2 []]()()[] Taking LCM and multiplying each by LCM, we get 6, 6 x (1/3) 6 x (1/2)

i.e., (6, 2, 3)

The miller indices of the plane ABC is (6 2 3)

Procedure for finding Miller indices:

- Find the intercepts of the plane along the coordinate axes X, Y, Z. Let these be (pa, q b, r c).
- Express the intercepts as multiples of the unit cell dimension (p, q, r)
- Take the reciprocal of these numbers 1/p, 1/q, 1/r.
- Convert these reciprocals into whole numbers by multiplying each with the LCM. Enclose these integers within bracket without commas.
- This gives the Miller indices (h K I) of the plane.

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7. (a) Describe Bridgman and Czochralski method of growing single crystals. What are the advantages and limitations of this method?

[OR]

(b) Describe the two bulk crystal growth methods in detail using suitable schematic diagrams to fabricate semiconductor and dielectric materials.

Bridgman technique of crystal growth of crystal.

Principle:

The selective cooling of the molten material to form single crystal by solidification along a particular direction.

Description:

 It consists of a vertical cylindrical crucible made of platinum and tapered conically with a pointed tip at the bottom.



- The crucible is surrounded by furnace 1 and furnace 2.
- The furnace coil winding is such that the upper zone is hotter than the lower zone.
- A pulley arrangement is made in order to move the crucible up and down during the crystallization process.

Working:



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- The material to be grown in the form of single crystal is taken in the crucible.
- The crucible is suspended in the upper furnace until the material gets melted completely into molten liquid.
- A crucible is slowly lowered from the hot zone to the cold zone. The movement should be in the range of 1mm per hour
- As the pointed tip enter the cold zone, the melt gets solidified
- As the crucible is lowered further, the growth continues and large single crystal is formed.

Advantage:

1)Relatively cheaper

2)Simple technology

3)Controlled growth

4) The thermal gradients can be easily minimized

Disadvantage:

1)Growth rate is very low

2)Sometime instead of single crystal, poly crystal may growth

Czochralski method of growing single crystal:

Principle:

It is a crystal pulling technique in which crystals are grown by gradual layer by layer condensation of melt initiated by a seed crystal.

Description:

- The apparatus consists of crucible, heater, seed crystal and crystal holder.
- The crucible is made up of graphite. It is provided with a heating element to heat the material into a melt.
- It is also consisting of a shaft for rotating and pulling the growing crystal.
- The rotating shaft has a seed holder in which the seed crystal is attached.
- The entire setup is kept inside a high vacuum chamber to avoid contamination and oxidation.

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Working:

- The raw material is taken in the crucible and is melted by means of the heating element.
- The material is heated above its melting point so that a clear melt is obtained.
- A small seed crystal of desired orientation is attached to the pulling rod and is lowered into the surface of the molten material.
- The seed touches the melt and gets slightly melted.
- Now the temperature is reduced below the melting point to permit atoms get attached to the seed crystal.
- The rod is now rotated about its axis and is drawn upwards slowly.
- The diameter of the crystal increases if the rod is pulled up slowly. The diameter decreases if the rod is pulled up quickly.
- When the crystal has reached its desired length, the temperature is lowered to room temperature and the crystal is raised quickly and withdrawn from the

