INDIAN INSTITUTE OF TECHNOLOGY ROORKEE
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Structural Analysis of Nanomaterials
LECTURE – 02
Structure of Materials
With
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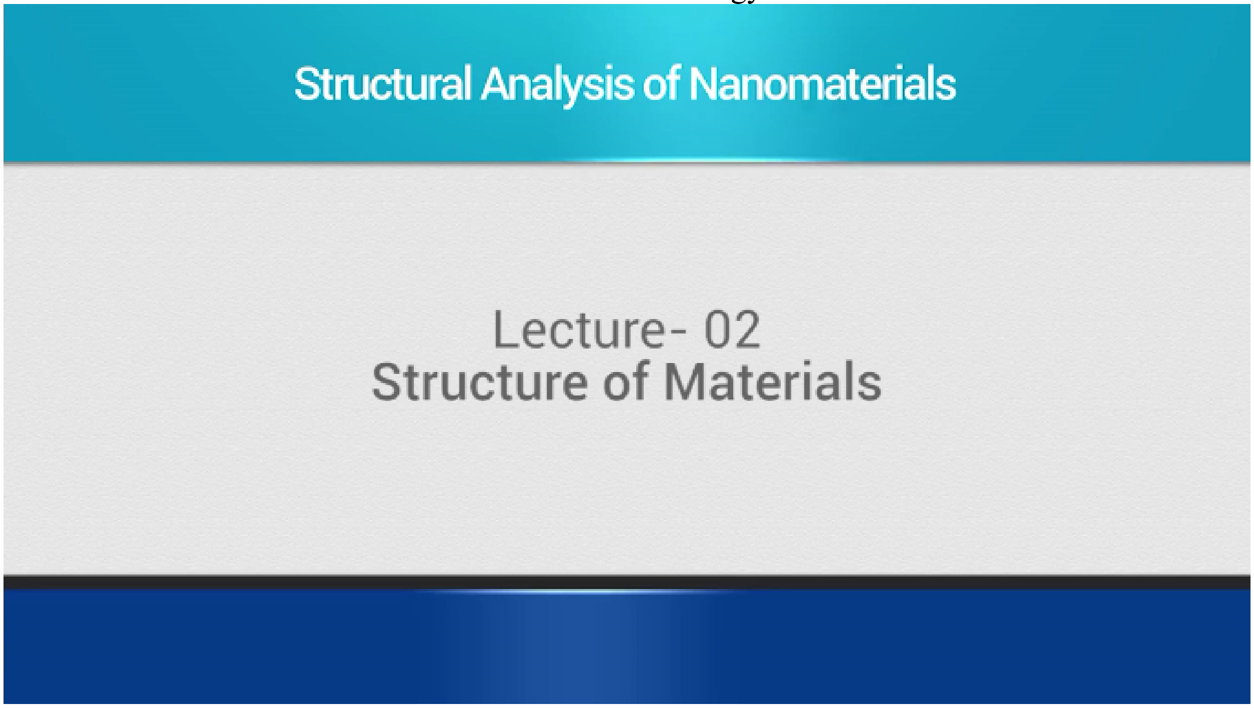

Structural Analysis of Nanomaterials

Lecture- 02
Structure of Materials

With

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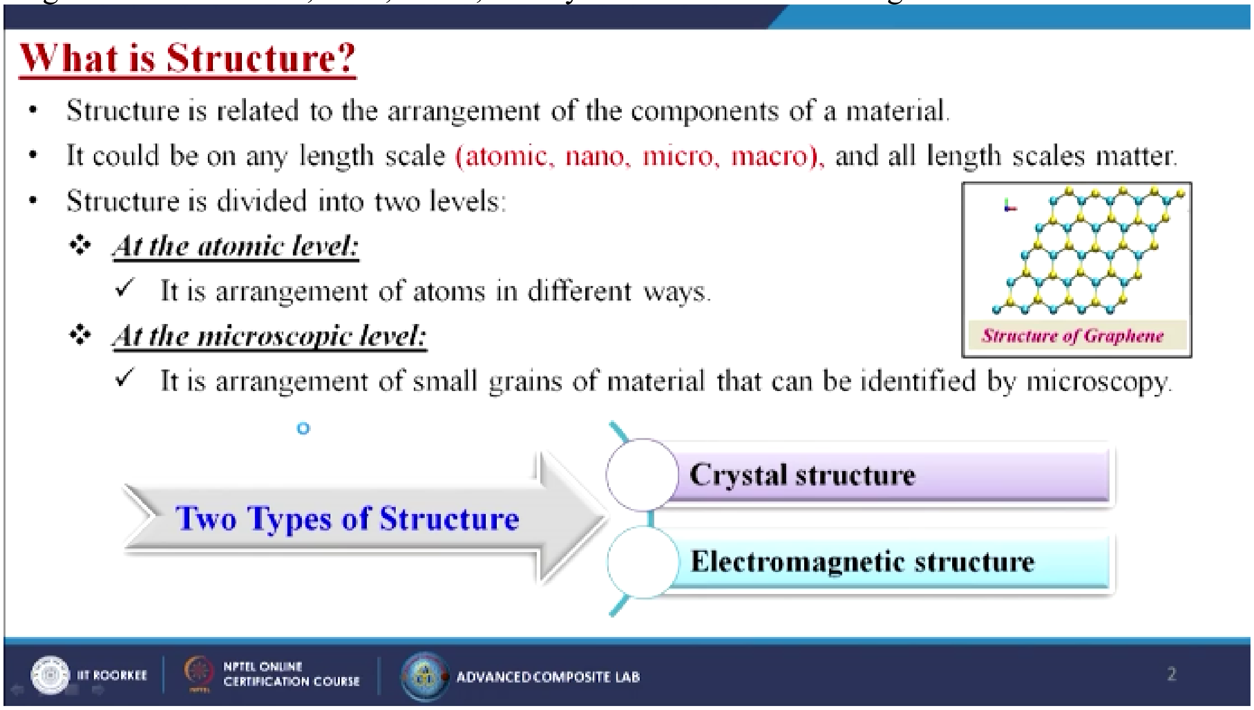
Today we are going to discuss about the structure of materials, if you remember in our last lecture we have already discussed about the atomic bonding and the atomic structure of different materials, so in this particular lecture we will only focus on the structure of materials.

So first let us know that what is structure, so structure is related to the arrangement of the components of a material that means it's the skeleton of any kind of material, it could be on any length scale like atomic, nano, micro, or maybe the macro and all length scales matter for structure. Structure generally we are dividing into two levels, first is called the atomic level and the second here is called the microscopic level.



What is Structure?

- Structure is related to the arrangement of the components of a material.
- It could be on any length scale (atomic, nano, micro, macro), and all length scales matter.
- Structure is divided into two levels:
  - ❖ ***At the atomic level:***
    - ✓ It is arrangement of atoms in different ways.
  - ❖ ***At the microscopic level:***
    - ✓ It is arrangement of small grains of material that can be identified by microscopy.

Structure of Graphene

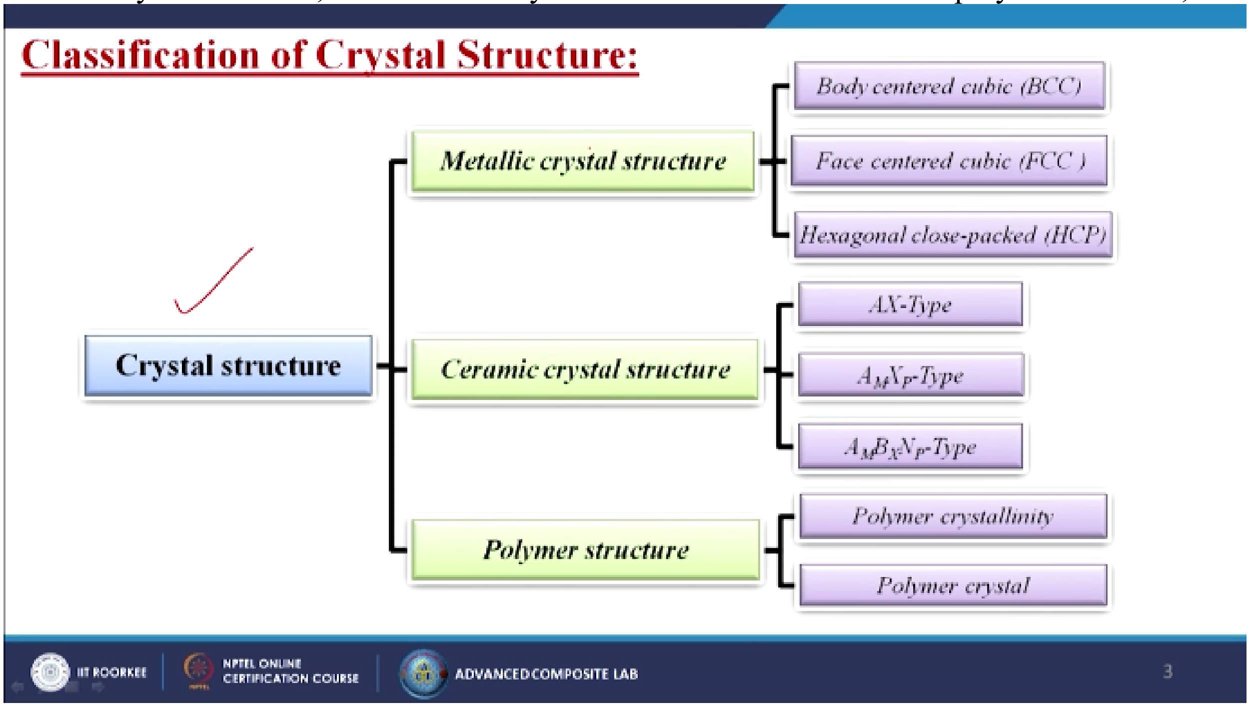
Two Types of Structure

Crystal structure

Electromagnetic structure

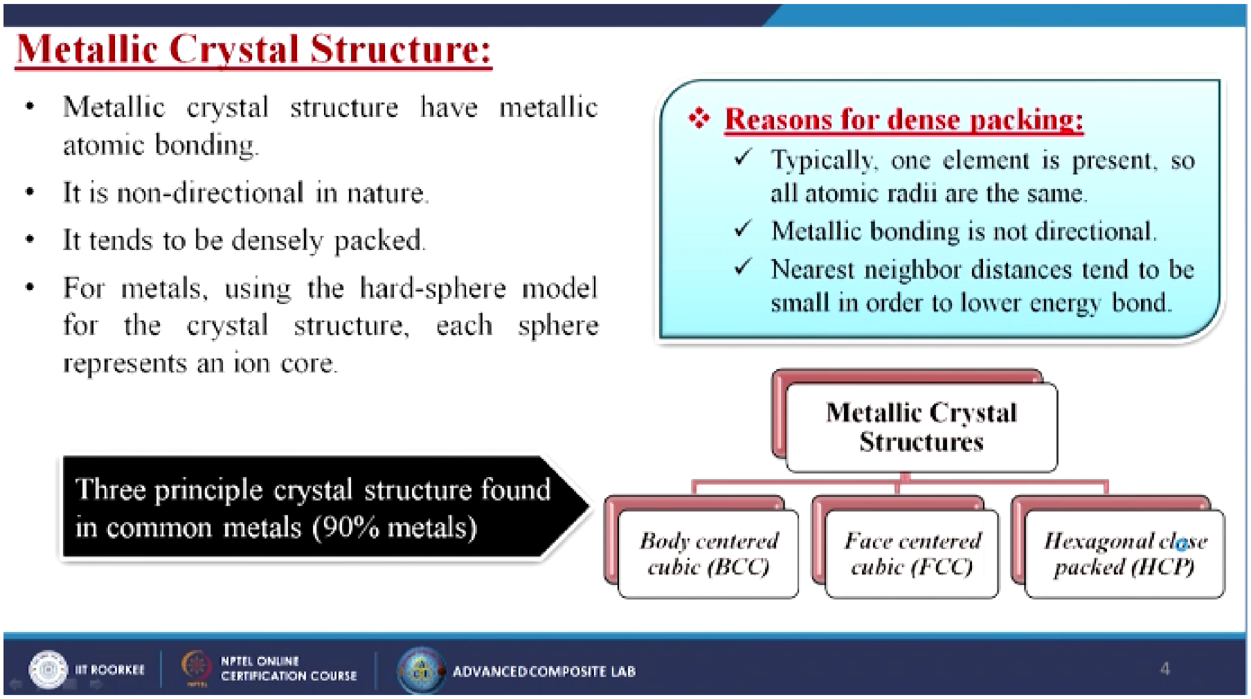
Atomic level which will give us the different arrangement of atoms in different ways and microscopic level that means it will give you the small grain of materials that can be identified by the microscopy either maybe it is optical microscopy or maybe scanning electron microscopy or maybe the transmission electron microscopy.

So generally there are two types of structure, first one is called the crystal structure and second one is called the electromagnetic structure. So if we do the classification of the crystal structure, so as I told already the crystal structure it will be divided into three parts one is called the metallic crystal structure, then ceramic crystal structure and last one is the polymer structure, so if we see the metallic crystal structure so we can find three types of structure, one is called the BCC or maybe the body centered cubic, then face centered cubic or maybe the FCC, and last one is the hexagonal closed packed or generally we are calling it as a HCP structure. When you are talking about the ceramic crystal structure generally it is AX-Type, AM XP Type, AM BX NP Type, and when we are talking about the polymer structure, so generally polymer crystallinity and polymer crystal.



Classification of Crystal Structure:

- **Crystal structure**
  - *Metallic crystal structure*
    - *Body centered cubic (BCC)*
    - *Face centered cubic (FCC)*
    - *Hexagonal close-packed (HCP)*
  - *Ceramic crystal structure*
    - *AX-Type*
    - $A_M X_P$*-Type*
    - $A_M B_X N_P$*-Type*
  - *Polymer structure*
    - *Polymer crystallinity*
    - *Polymer crystal*



Metallic Crystal Structure:

- Metallic crystal structure have metallic atomic bonding.
- It is non-directional in nature.
- It tends to be densely packed.
- For metals, using the hard-sphere model for the crystal structure, each sphere represents an ion core.

❖ **Reasons for dense packing:**

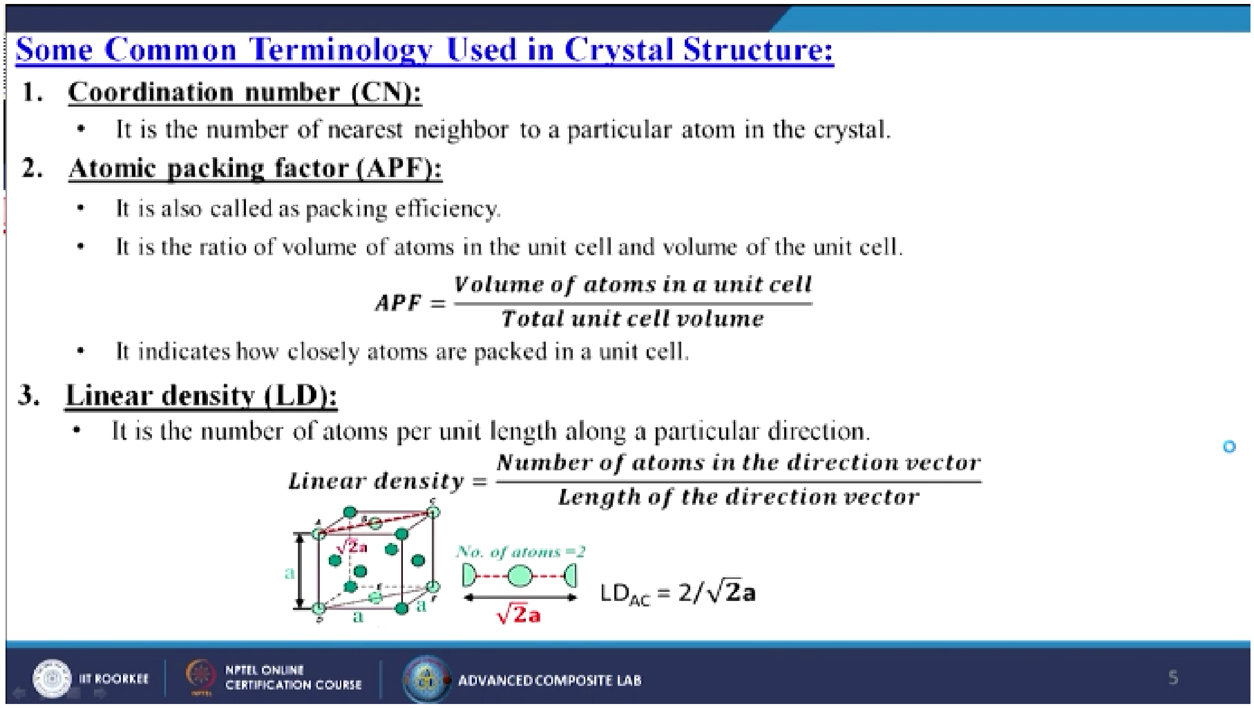
- ✓ Typically, one element is present, so all atomic radii are the same.
- ✓ Metallic bonding is not directional.
- ✓ Nearest neighbor distances tend to be small in order to lower energy bond.

Three principle crystal structure found in common metals (90% metals)

Metallic Crystal Structures

- *Body centered cubic (BCC)*
- *Face centered cubic (FCC)*
- *Hexagonal close packed (HCP)*

So now first let us discuss about the metallic crystal structure, so generally the metallic crystal structure have metallic atomic bonding so that's why it's known as the metallic crystal structure, so it is non-directional in nature, it tends to be very densely or maybe the closely packed the gap in between the atoms is very very less, for metals generally using the hard sphere model for the crystal structure, each sphere represents an ion core, so what is the reason for the dense packing? So generally one element is present so all atomic radius are the same, metallic bonding is not directional, and last one is that nearest neighbor distances tends to be small in order to lower the energy bond, so there are mainly 3 principle crystal structure found in the common metals more or less 90% of metals, one is called the body centered cubic, then face centered cubic and the hexagonal closed packed.



Some Common Terminology Used in Crystal Structure:

1. **Coordination number (CN):**
   - It is the number of nearest neighbor to a particular atom in the crystal.
2. **Atomic packing factor (APF):**
   - It is also called as packing efficiency.
   - It is the ratio of volume of atoms in the unit cell and volume of the unit cell.

$$APF = \frac{Volume\ of\ atoms\ in\ a\ unit\ cell}{Total\ unit\ cell\ volume}$$

   - It indicates how closely atoms are packed in a unit cell.
3. **Linear density (LD):**
   - It is the number of atoms per unit length along a particular direction.

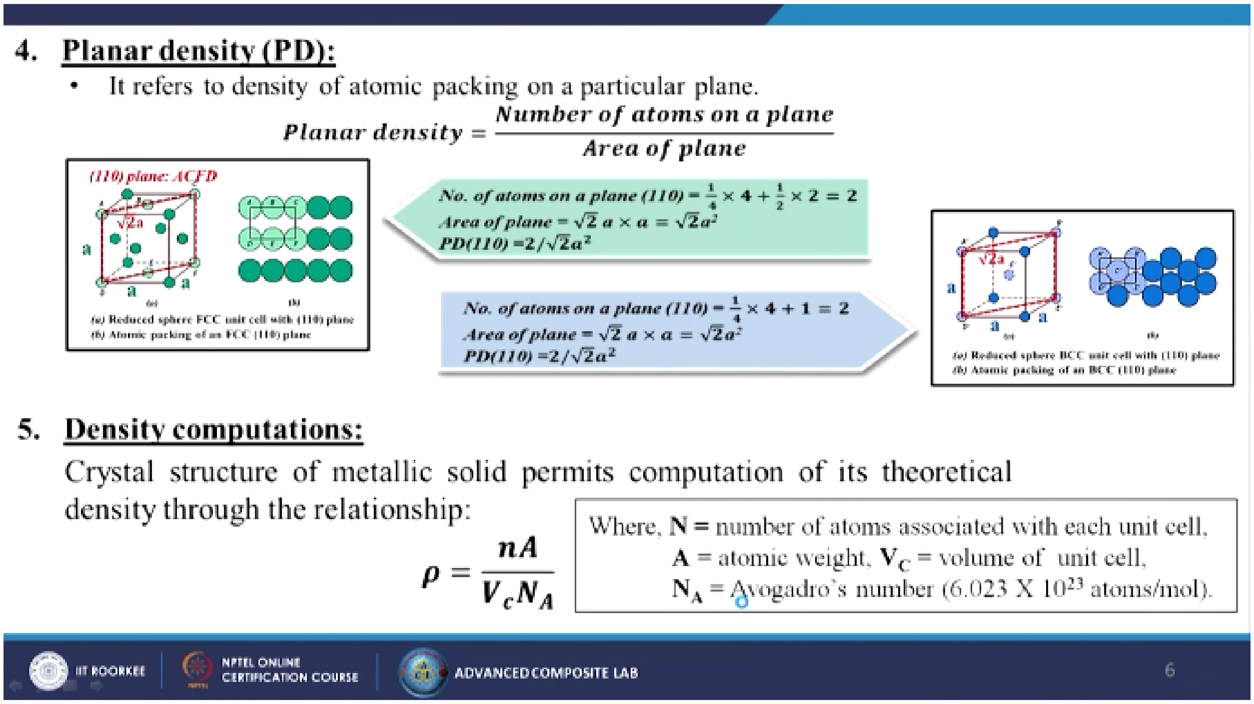
$$Linear\ density = \frac{Number\ of\ atoms\ in\ the\ direction\ vector}{Length\ of\ the\ direction\ vector}$$

So now let us discuss about the some common terminology that generally which we are using for the determining the crystal structure, so first is called the coordination number or maybe in short we are calling it as a CN, so what is that? It is the number of nearest neighbor to a particular atom in the crystals, so nearest neighboring, how many partners or maybe atoms are present over there that is known as the coordination number.

Next is known as the atomic packing factor, this is very very important one, so it is also called as a packing efficiency also, so it is the ratio of volume of atoms in the unit cell and volume of the unit cell, so generally we are giving atomic packing factor is also known as, in short terms is called the APF, so what is APF? Volume of atoms in a unit cell divided by total unit cell volume, generally it indicates how closely atoms are packed in a unit cell.

Next we are going to know another term that is called the linear density, so it is the number of atoms per unit length along a particular directions, so linear density is generally number of atoms in the direction vector by length of the direction vector, so in this case you see so when we are talking about we are having A and C point and then what is the length of the direction vector? It is root over 2A because it is the cubic structure so all the sides are A, so automatically this A to C is known as the root over 2A.

Now what are the number of atoms over there, if you see it that it is half of that one then one single and another half so total number of atoms is 2, so what is the linear density over here? That is 2/root over 2A, so another important term is called the planar density, so generally planar density sometimes it is called as a PD, so it refers to density of atomic packing on a particular



4. Planar density (PD):

- It refers to density of atomic packing on a particular plane.

$$\textit{Planar density} = \frac{\textit{Number of atoms on a plane}}{\textit{Area of plane}}$$

(110) plane: ACFD

(a) Reduced sphere FCC unit cell with (110) plane
(b) Atomic packing of an FCC (110) plane

No. of atoms on a plane (110) = $\frac{1}{4} \times 4 + \frac{1}{2} \times 2 = 2$
Area of plane = $\sqrt{2}\, a \times a = \sqrt{2}a^2$
PD(110) = $2/\sqrt{2}a^2$

No. of atoms on a plane (110) = $\frac{1}{4} \times 4 + 1 = 2$
Area of plane = $\sqrt{2}\, a \times a = \sqrt{2}a^2$
PD(110) = $2/\sqrt{2}a^2$

(a) Reduced sphere BCC unit cell with (110) plane
(b) Atomic packing of an BCC (110) plane

5. Density computations:

Crystal structure of metallic solid permits computation of its theoretical density through the relationship:

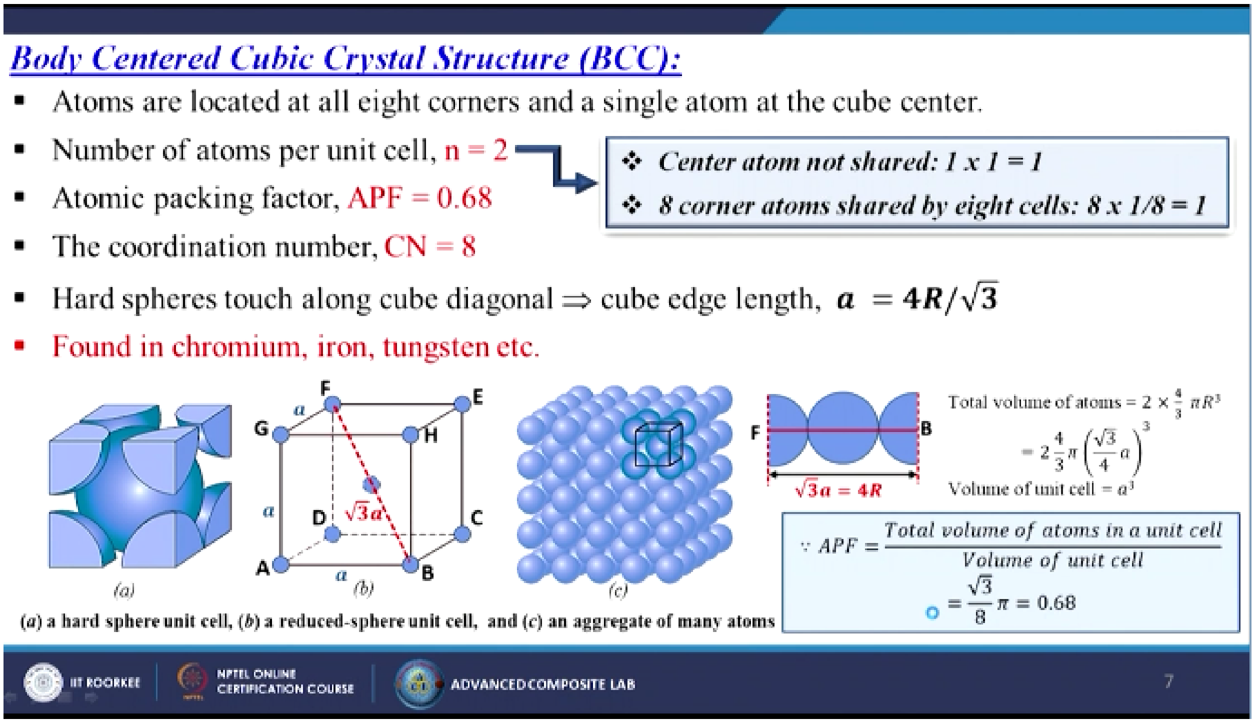
$$\rho = \frac{nA}{V_c N_A}$$

Where, **N** = number of atoms associated with each unit cell,
A = atomic weight, $\mathbf{V_C}$ = volume of unit cell,
$\mathbf{N_A}$ = Avogadro's number (6.023 X 10^{23} atoms/mol).

plane, so generally planar density number of atoms on a plane by area of a plane, so when you are talking about a 1 1 0 plane so generally if you see that is also a cubic structure, so here 1 1 0 plane is nothing but the plane is consist of A, C, F and D, so if any cube we just, we make it a cross section and just corner to corner, so in this particular case what are the number of atoms on a plane, it's 1/4 x 4 + 1/2 x 2, so that total number of atoms present are 2, because this 4 so 1/4 of that part, so 1/4 x 4 and this one B point is 1/2 and E point is the 1/2 one, so total number of atoms is 2.

And what is the area of plane? Root over 2A because this is A to C is root over, A to C is root over 2A into the height that means A, so root over 2A square, so the planar density along the plane 1 1 0 is 2/root over 2A square, now if we talk about the BCC structure, so here the number of atoms on a plane 1 1 0 is 1/4 x 4 because 1, 2, 3, 4, A prime, B prime, E prime, D prime, so 1/4 x 4 + 1 is into the middle, so that is the C prime, so here is also the number of atoms is 2, area of plane it should be root over 2A x A, because A prime to B prime is also here root over 2A.

Now what is the planar density? 1 1 0 plane, it's 2/root over 2A square. Now we are going to discuss about the density computations, so crystal structure of metallic solid permits the computations of its theoretical density through this relationships which is nothing but the row is equal to NA/VC NA, what is capital N over here? N is nothing but the number of atoms associated with each unit cell, what is A? A is the atomic weight, what is VC? That is volume of unit cell. What is NA? That is nothing but the Avogadro's number that is 6.023 x 10 to the power 23 atoms per mole.



Body Centered Cubic Crystal Structure (BCC):

- Atoms are located at all eight corners and a single atom at the cube center.
- Number of atoms per unit cell, n = 2
- Atomic packing factor, APF = 0.68
- The coordination number, CN = 8
- Hard spheres touch along cube diagonal ⇒ cube edge length, $a = 4R/\sqrt{3}$
- Found in chromium, iron, tungsten etc.

❖ *Center atom not shared: 1 x 1 = 1*

❖ *8 corner atoms shared by eight cells: 8 x 1/8 = 1*

(a) (b) (c)

(*a*) a hard sphere unit cell, (*b*) a reduced-sphere unit cell, and (*c*) an aggregate of many atoms

$$\text{Total volume of atoms} = 2\times\frac{4}{3}\pi R^3 = 2\frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3$$

$$\text{Volume of unit cell} = a^3$$

$$\because APF = \frac{\textit{Total volume of atoms in a unit cell}}{\textit{Volume of unit cell}} = \frac{\sqrt{3}}{8}\pi = 0.68$$

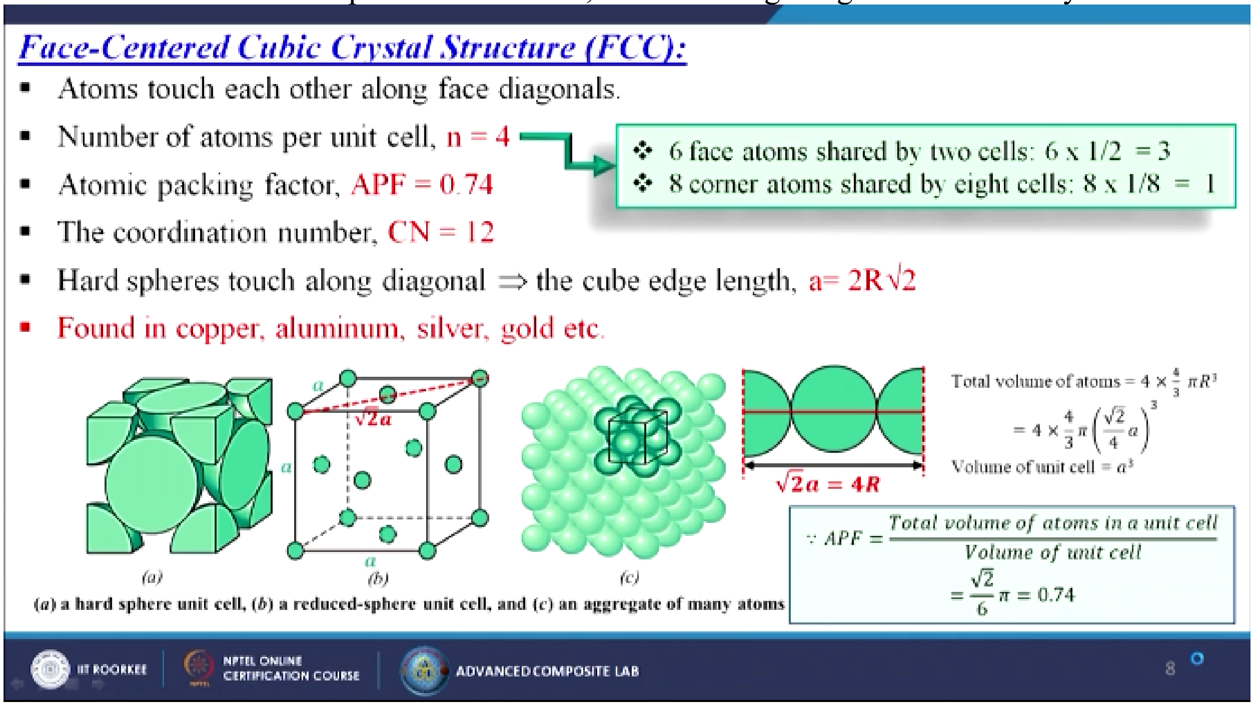
Now we are going to discuss about the body centered cubic crystal structure, so in this particular crystal structures atoms are located at all 8 corners, so from this figure, this B figure you can see that atoms are located all the 8 corners over there, and the single atom at the cube center so this one, so total number of atoms per unit cell is equal to 2, already we have gone through in our last slides, because the center atom not shared that is 1 x 1 that is 1, and 8 corners atom shared by the 8 cells that is 8 x 1/8 that is 1, so 1 + 1 = 2.

What is the atomic packing factor over there? So generally atomic packing factor is 0.68, how we are calculating this one? If we clearly see this image, so you can find that from F to B so automatically there is one half atom, one full atom, and another half atom, so if I take the radius of the atom is R, so total distance is 4R, which is nothing but the root over 3A because in a cubic systems if all the sides are A so automatically F to B will be root over 3A, so root over 3A = 4R.

So now what is the total volume of the atoms? That is 2 x 4/3 pie R cube = 2 x 4/3 pie and if I put the value of R over here which is nothing but the root over 3/4A to the power cube, so volume and here also the volume of unit cell is A cube, so volume and here also the volume of unit cell is A cube, so now what is the atomic packing factor? Because atomic packing factor we know total volume of the atoms in the unit cell by the volume of the unit cell, so it should be this divided by this, so what we are getting actually finally? Root over 3/8 pi which is nothing but the 0.068.

What is the coordination number over here? That is 8, hard spheres generally tough along cube diagonals, so cube edge length, if I want to calculate the A so generally the A value is equal to 4R/root over 3, so same we are getting from this particular dimensions, so generally it can be found in chromium, iron, or tungsten.

Now we are going to discuss about the face centered cubic crystal structure or it may be in short generally we are calling it as a FCC structure, so atom touch each other along face diagonals,



Face-Centered Cubic Crystal Structure (FCC):

- Atoms touch each other along face diagonals.
- Number of atoms per unit cell, n = 4
- Atomic packing factor, APF = 0.74
- The coordination number, CN = 12
- Hard spheres touch along diagonal ⇒ the cube edge length, a= 2R√2
- Found in copper, aluminum, silver, gold etc.

❖ 6 face atoms shared by two cells: 6 x 1/2 = 3
❖ 8 corner atoms shared by eight cells: 8 x 1/8 = 1

(a) a hard sphere unit cell, (b) a reduced-sphere unit cell, and (c) an aggregate of many atoms

$\sqrt{2}a = 4R$

Total volume of atoms $= 4 \times \frac{4}{3}\pi R^3$

$= 4 \times \frac{4}{3}\pi\left(\frac{\sqrt{2}}{4}a\right)^3$

Volume of unit cell $= a^3$

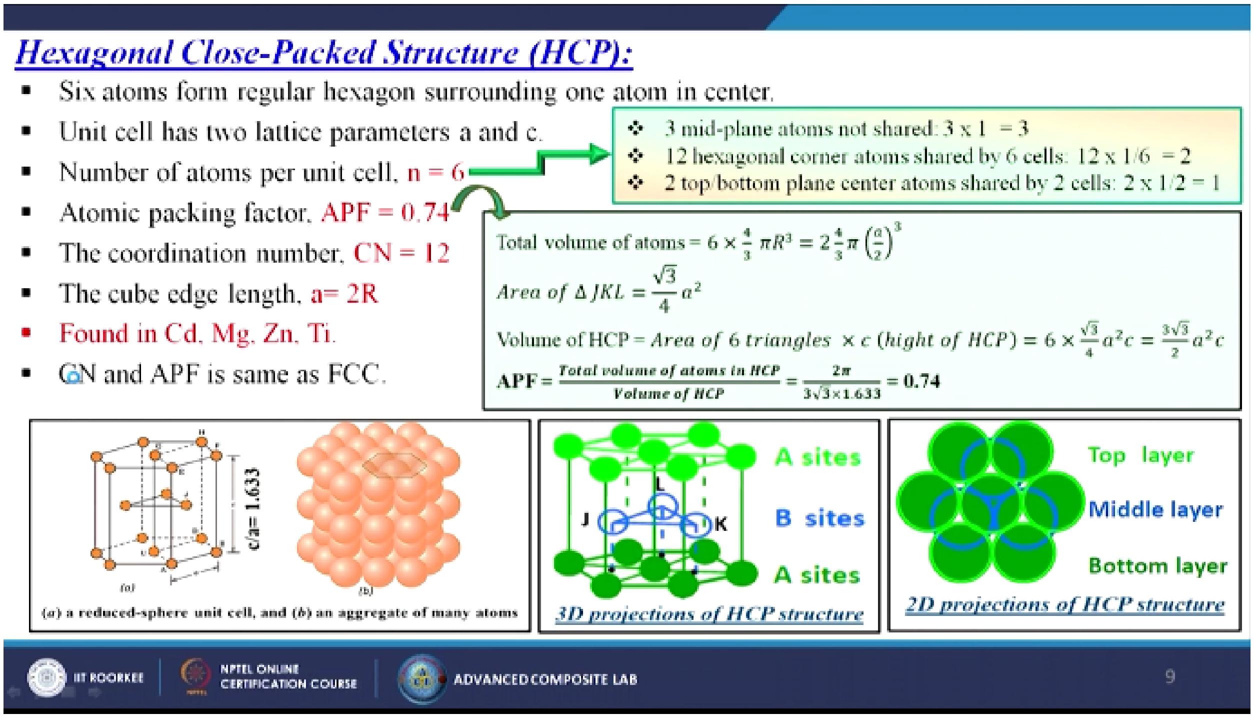
$$\because APF = \frac{\textit{Total volume of atoms in a unit cell}}{\textit{Volume of unit cell}} = \frac{\sqrt{2}}{6}\pi = 0.74$$

here the number of atoms per unit cell n = 4, how we are getting this one? So if you see this B figure over here so you can see all the corners we are having one one atoms then all the faces we are having one one atoms, so six face atoms shared by the two cells that is, that's why 6 x 1/2 = 3, and 8 corner atoms shared by the 8 cells 8 x 1/8 = 1, so 3 + 1 = 4, so total number of atoms per unit cell is 4.

So now what is the atomic packing factor over there? So if you see then we are doing the same thing, now we are just going to take the distance from this point to this point, so what is that? Same thing, it's half then full and then half, so R, then 2R, and R, so total it is 4R, so 4R = root over 2A because this is the root over 2A.

So now how it is possible? If all the sides dimensions are A, and all are perpendicular to each other for a cubic system so automatically this will be root over 2A, so root over 2A = 4R. So now total volumes of atoms is equal to 4 x 4/3 pi R cube which is nothing but the 4 x 4/3 pi and just we are replacing the R value over there which is nothing but root over 2/4R, A value just, we are putting the R value root over 2A by the 4, so we are putting over here and then whole cube, and here the volume of the unit cell is A cube, so what is the atomic packing factor over here? Same thing total volume of atoms in unit cell by volume of unit cell which is nothing but root over 2/6 pi which is nothing but the 0.74 whatever we have written over here.

So what is the coordination number over here? The coordination number is 12, hard spheres touch along diagonal, the cube edge length is A = 2R root over 2, then generally it can be FCC structure can be found in copper, aluminum, silver, gold, etcetera.



Hexagonal Close-Packed Structure (HCP):

- Six atoms form regular hexagon surrounding one atom in center.
- Unit cell has two lattice parameters a and c.
- Number of atoms per unit cell, n = 6
- Atomic packing factor, APF = 0.74
- The coordination number, CN = 12
- The cube edge length, a= 2R
- Found in Cd, Mg, Zn, Ti.
- CN and APF is same as FCC.

- 3 mid-plane atoms not shared: 3 x 1 = 3
- 12 hexagonal corner atoms shared by 6 cells: 12 x 1/6 = 2
- 2 top/bottom plane center atoms shared by 2 cells: 2 x 1/2 = 1

Total volume of atoms $= 6 \times \frac{4}{3}\pi R^3 = 2\frac{4}{3}\pi\left(\frac{a}{2}\right)^3$

$Area\ of\ \Delta JKL = \frac{\sqrt{3}}{4}a^2$

Volume of HCP $= Area\ of\ 6\ triangles\ \times c\ (hight\ of\ HCP) = 6 \times \frac{\sqrt{3}}{4}a^2c = \frac{3\sqrt{3}}{2}a^2c$

$\mathbf{APF} = \frac{Total\ volume\ of\ atoms\ in\ HCP}{Volume\ of\ HCP} = \frac{2\pi}{3\sqrt{3}\times 1.633} = \mathbf{0.74}$

(a) a reduced-sphere unit cell, and (b) an aggregate of many atoms

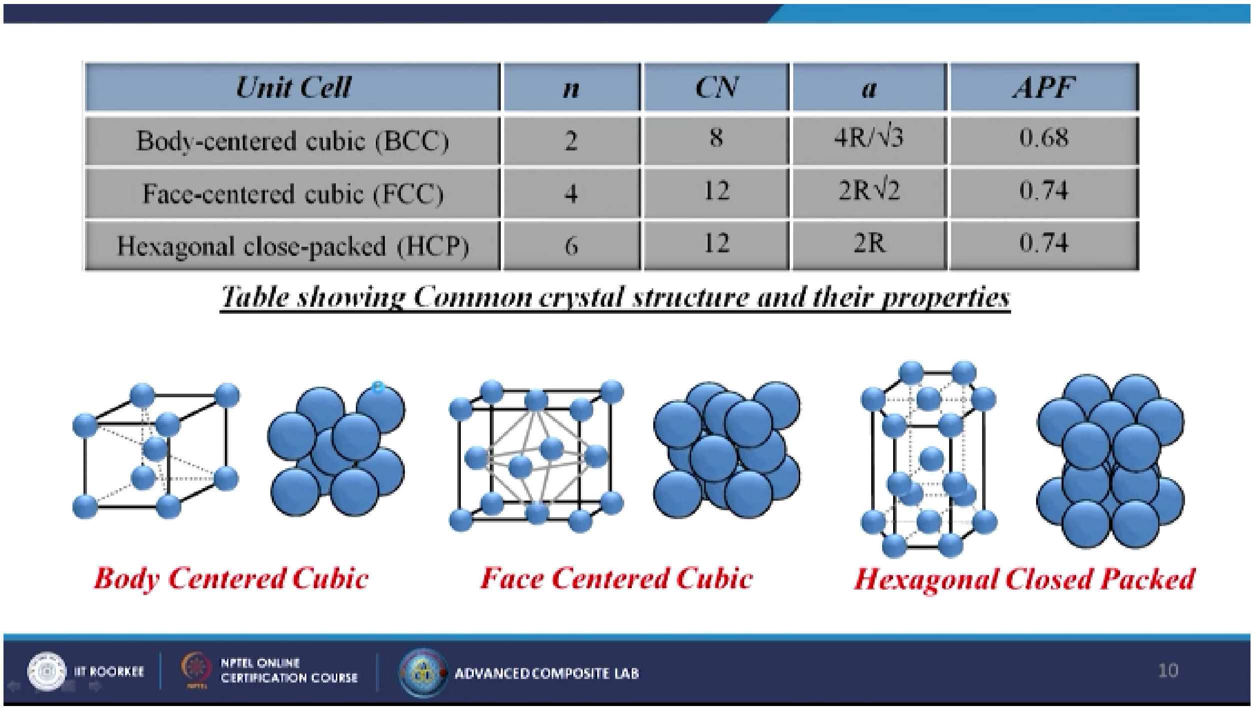
3D projections of HCP structure

2D projections of HCP structure

Now we are going to discuss about the hexagonal close packed structure, so generally 6 atoms form regular hexagon surrounding one atom in center you can see from this particular image, unit cell has two lattice parameters here, one is called the A, another one is the C, so A is the distance between A to B, and from B to A the distance is C. What is the number of atoms per unit cell? N = 6, how we are getting it? 3 mid plane atoms not shared so it's directly 3 x 1 = 3, 12 hexagonal corner atoms shared by the 6 cells, so 12 x 1/6 that is 2, and then two top bottom plane center atom shared by the two cells so that's why 2 x 1/2 = 1, so 3 + 2 + 1, so that means total 6.

Now how we are going to calculate the atomic packing factor over there? So for this you have to see this picture, in this picture you can find that we have gone through this triangle shapes J, K and L, so the triangle JKL total volume of atoms, what is that? 6 x 4/3 pi R cube which is 2 x 4/3 pi x A/2 whole cube, so what is the area of this JKL triangle? It is root over 3/4A square, what is the volume of that HCP? Area of 6 triangles into C, C means this one, height of HCP which is nothing but the 6 x root over 3/4 A square C = 3 root over 3/2 A square C, so what is the APF value over there? Total volume of atoms in HCP by volume of HCP which is nothing but the 2 pi/3 root over 3 x 1.633, which is nothing but 0.74 over there.

What is the coordination number? So here the coordination number is 12, the cube edge length A is equal to generally 2R, found in generally cadmium, magnesium, zinc, titanium, here coordination number and atomic packing factor is same as FCC.

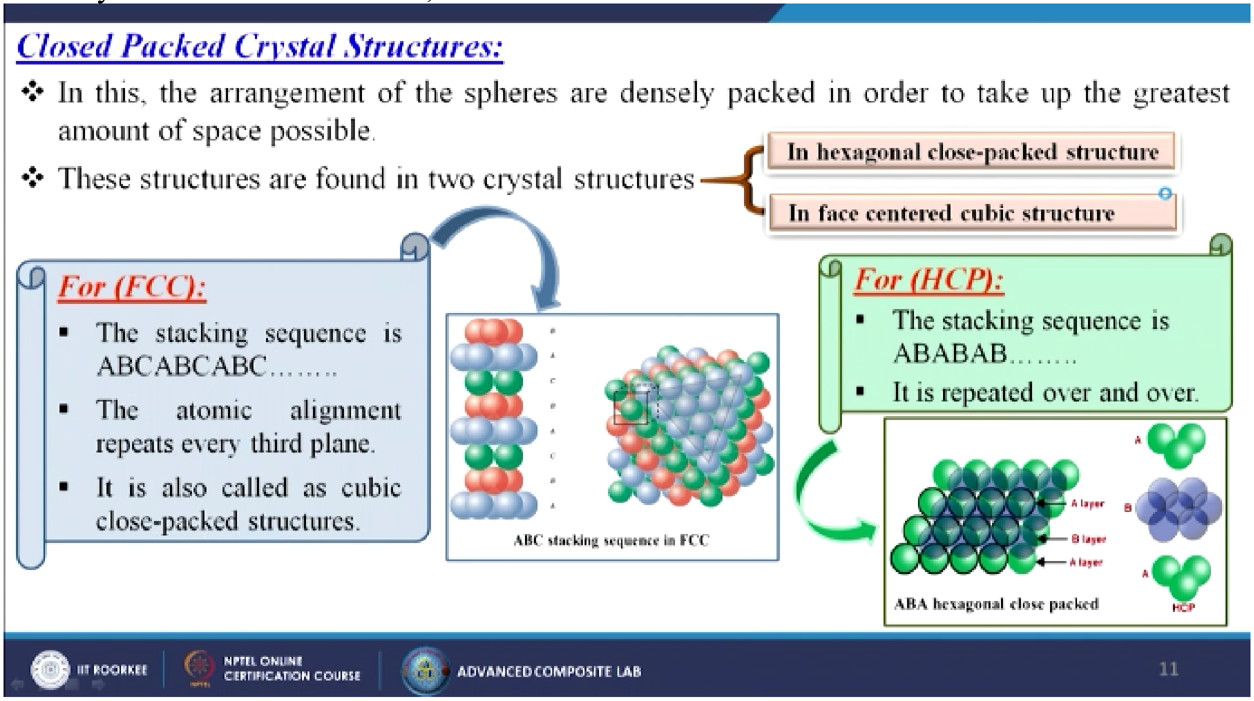


Unit Cell	n	CN	a	APF
Body-centered cubic (BCC)	2	8	4R/√3	0.68
Face-centered cubic (FCC)	4	12	2R√2	0.74
Hexagonal close-packed (HCP)	6	12	2R	0.74

Table showing Common crystal structure and their properties

Body Centered Cubic **Face Centered Cubic** **Hexagonal Closed Packed**

Now this is the overall comparisons, so for generally unit cell as I told already we have given body centered cubic, face centered cubic and hexagonal closed packed, so herein is equal to the unit cell number is 2 for the BCC, 4 for the FCC, and 6 for the HCP, what is the CN number over here for 8, 12, and 12, what is the A? That is the lattice parameter, for body centered cubic it is 4R/root over 3 and R is the radius of that particular atom, face centered cubic it is 2R root over 2, and then for hexagonal closed packed it is 2R, and what is the atomic packing factor number? So for body centered cubic it is 0.68, for face centered cubic it is 0.74 and for HCP it is 0.74 also.



Closed Packed Crystal Structures:

- In this, the arrangement of the spheres are densely packed in order to take up the greatest amount of space possible.
- These structures are found in two crystal structures
  - In hexagonal close-packed structure
  - In face centered cubic structure

For (FCC):

- The stacking sequence is ABCABCABC……..
- The atomic alignment repeats every third plane.
- It is also called as cubic close-packed structures.

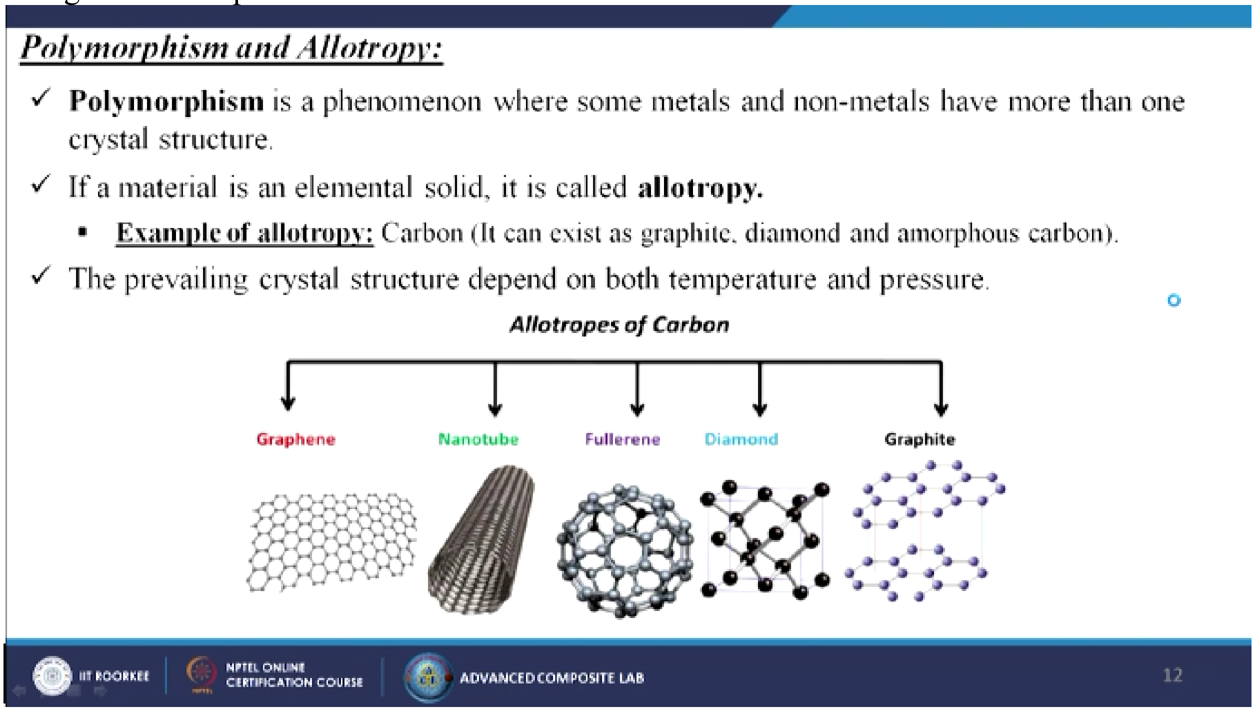
ABC stacking sequence in FCC

For (HCP):

- The stacking sequence is ABABAB……..
- It is repeated over and over.

ABA hexagonal close packed

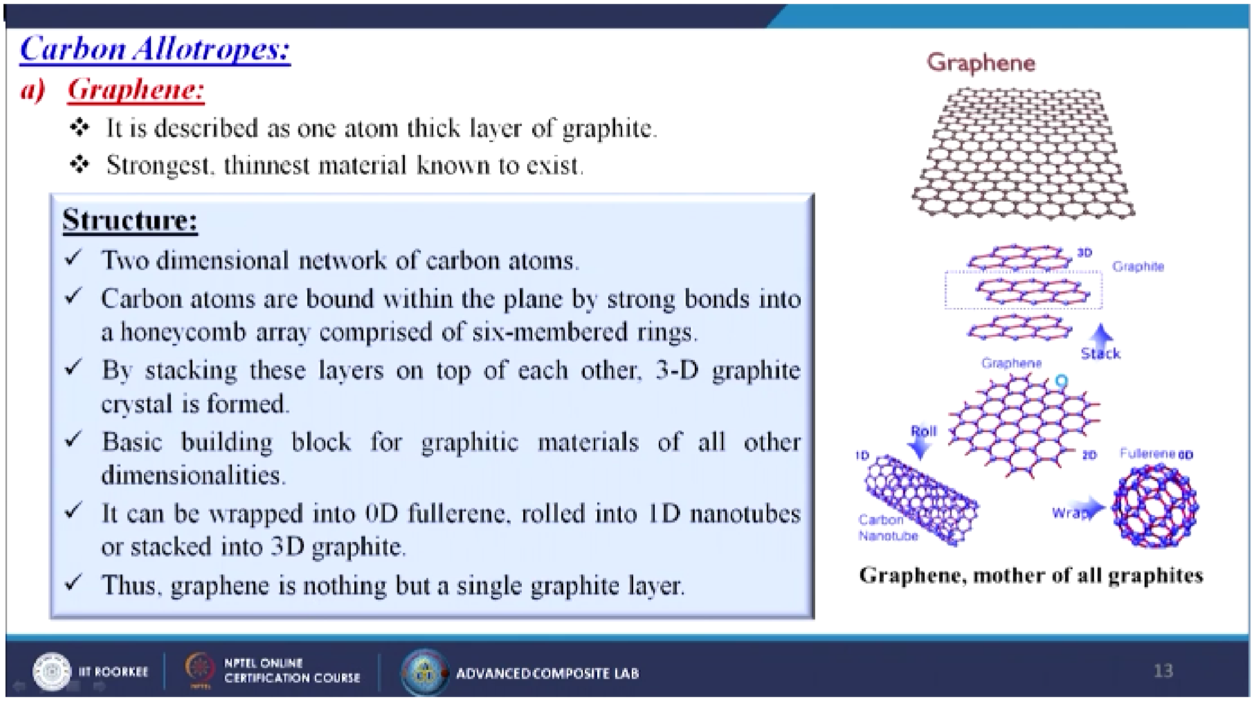
Now we are going to discuss about the closed packed crystal structures, so in this the arrangement of the spheres are densely packed in order to take up the greatest amount of space available, so very very close densely packed, these structures are found in two crystal structures, in hexagonal closed packed structure and another one is in face centered cubic structure, so for FCC generally the stacking sequence is like this, ABC and then ABC and then ABC, so if you find that after ABC again the repeating cell is coming over here, that same thing has been written, the atomic alignment repeats every third plane, it is also called as cubic close packed structure also, when we are talking about the HCP, so hexagonal closed packed the stacking sequence is ABABAB like that, so it's a layer by layer structure, so generally A, then after that B will come, then after that again A will come then after that again B will come, so this is the hexagonal closed packed structure.



Polymorphism and Allotropy:

- ✓ **Polymorphism** is a phenomenon where some metals and non-metals have more than one crystal structure.
- ✓ If a material is an elemental solid, it is called **allotropy.**
  - **Example of allotropy:** Carbon (It can exist as graphite, diamond and amorphous carbon).
- ✓ The prevailing crystal structure depend on both temperature and pressure.

Now we are going to discuss about the polymorphism and allotropy, so what is polymorphism? So polymorphism is a phenomenon where some metals and non-metals have more than 1 crystal structure, I'll give you this example so that you can better understand, so if a material is an element solid, it is called the allotropy, so what is the example of the allotropy? So generally the best example is the carbon, it can exist as a graphite, as a diamond, as a amorphous carbon, so it can be present into the environment in its so many forms, the prevailing crystal structure depend on both temperature and pressure, so what is the allotropes of carbon generally we can see graphene, we can see nanotube, we can see fullerene, we can see diamond, and we can see the graphite.



Carbon Allotropes:

a) Graphene:

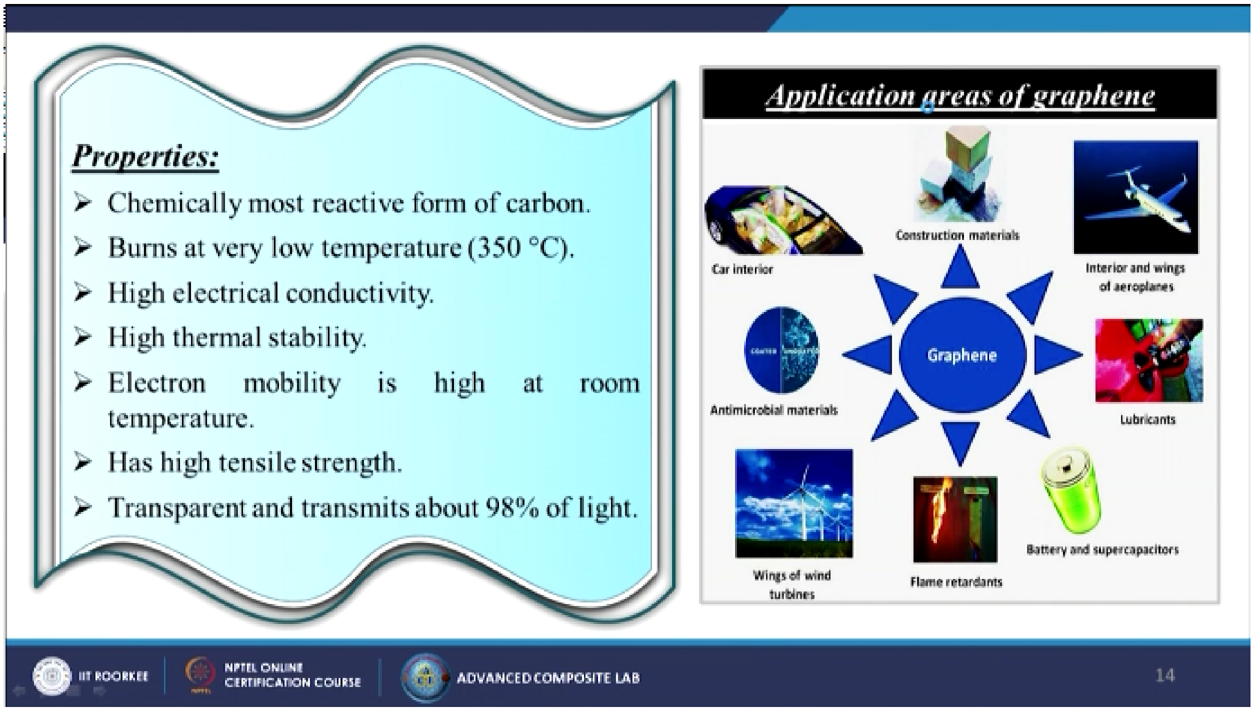
- It is described as one atom thick layer of graphite.
- Strongest, thinnest material known to exist.

Structure:

- ✓ Two dimensional network of carbon atoms.
- ✓ Carbon atoms are bound within the plane by strong bonds into a honeycomb array comprised of six-membered rings.
- ✓ By stacking these layers on top of each other, 3-D graphite crystal is formed.
- ✓ Basic building block for graphitic materials of all other dimensionalities.
- ✓ It can be wrapped into 0D fullerene, rolled into 1D nanotubes or stacked into 3D graphite.
- ✓ Thus, graphene is nothing but a single graphite layer.

Graphene, mother of all graphites

So now let us discuss one by one about the carbon allotropes, so first we are going to discuss about the graphene, so what is graphene? It is described as one atom thick layer of the graphite, strongest, thinnest material known to exist after diamond. Structure generally two dimensional network of carbon atoms are there, carbon atoms are bound within the plane by strong bond into a honeycomb array comprised of six membered rings, so here you can see that six membered rings and it is forming one graphene atom, so by stacking this layers on top of each other one 3D graphite crystal is formed, basic building block for graphitic materials of all other dimensionalities, it can be wrapped into 0D, then we are calling it as a fullerene, rolled into 1D, we are calling it as a nanotubes or stacked into 3D that is the graphite, so generally the graphene is 2D in nature, so thus graphene is nothing but a single graphite layer, so you can see that in this particular image there are stack of layers which is nothing but known as the graphite and then a single layer just we are calling it as a graphene.

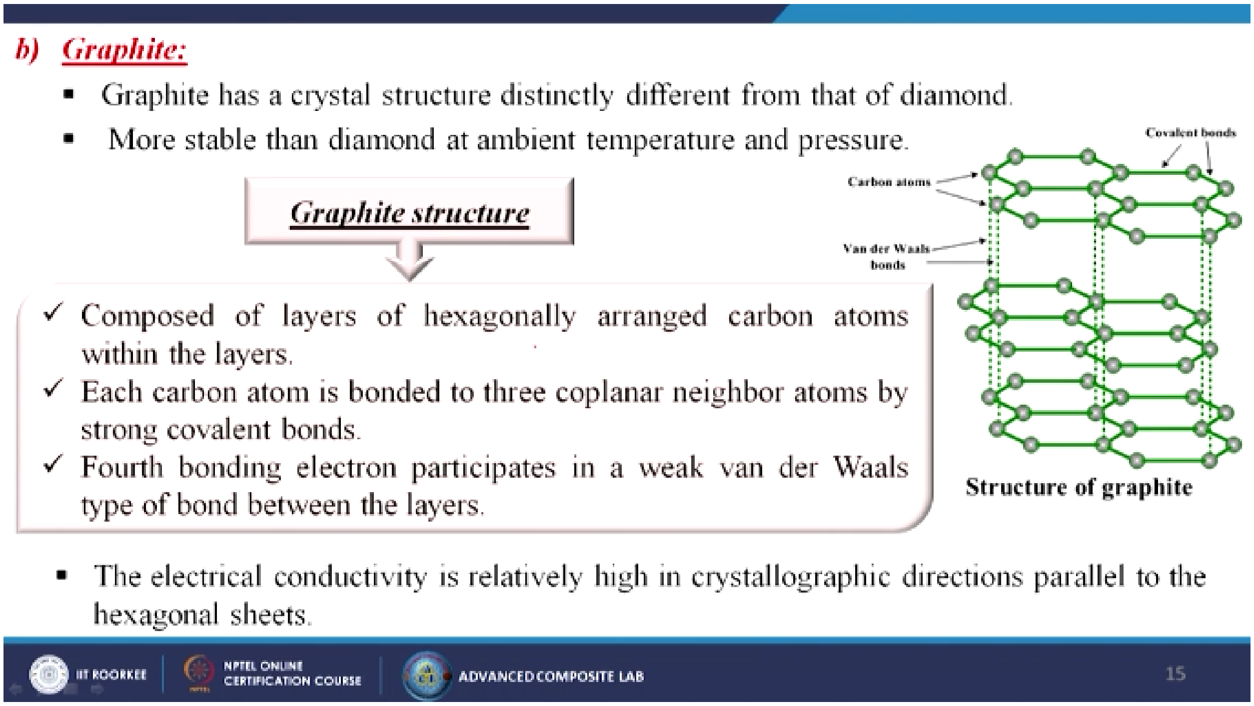


Properties:

- Chemically most reactive form of carbon.
- Burns at very low temperature (350 °C).
- High electrical conductivity.
- High thermal stability.
- Electron mobility is high at room temperature.
- Has high tensile strength.
- Transparent and transmits about 98% of light.

Application areas of graphene

Now what are the properties? Chemically most reactive form of carbon, burns at very low temperature generally 350 degree centigrade, high electrical conductivity, high thermal stability, high electron mobility at room temperature, high tensile strength, it's transparent and transmits about 98% of the light, so that's why it is the latest materials the whole researcher or maybe people are working on it, but still there are lots of things are still uncovered about the graphene, what are the application areas of the graphene, generally there are n number of applications nowadays where we are using the graphene, so in a brief idea we are using it for the automobile industry, for the construction materials, for the aerospace industry, for lubricants, for the battery super capacitor or maybe energy storage device then flame retardant materials, then turbines and then also for the biomedical applications like antimicrobial materials nowadays we are using for the scaffold, nowadays we are using for the orthopedic implants, so there are n number of applications where we are using the graphene.



b) Graphite:

- Graphite has a crystal structure distinctly different from that of diamond.
- More stable than diamond at ambient temperature and pressure.

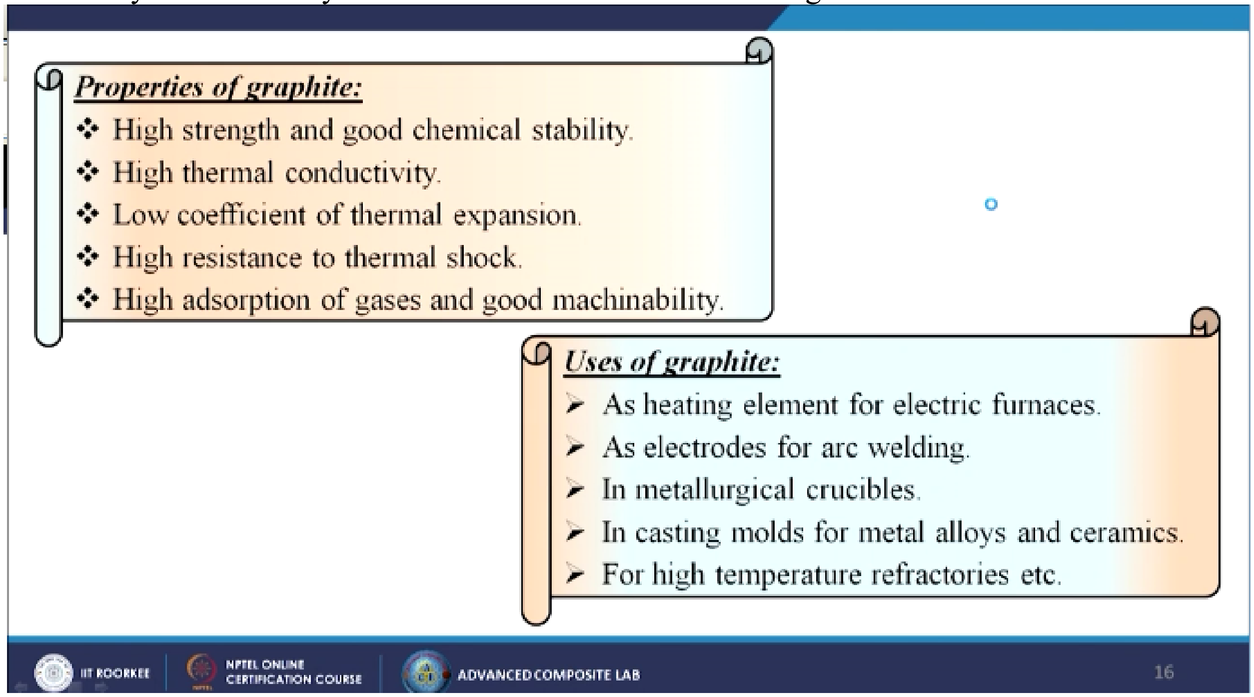
Graphite structure

- ✓ Composed of layers of hexagonally arranged carbon atoms within the layers.
- ✓ Each carbon atom is bonded to three coplanar neighbor atoms by strong covalent bonds.
- ✓ Fourth bonding electron participates in a weak van der Waals type of bond between the layers.

Structure of graphite

- The electrical conductivity is relatively high in crystallographic directions parallel to the hexagonal sheets.

So what is graphite? So graphite has a crystal structure distinctly different from that of diamond, most stable then diamond at ambient temperature and pressure, what is the graphite structure? Composed of layers of hexagonally arranged carbon atoms within the layers, each carbon atom is bonded to three coplanar neighbor atoms by strong covalent bonds, fourth bonding electron participates in a weak Van der Waals type of bond between the layers, so the electrical conductivity is relatively high in crystallographic directions parallel to the hexagonal sheets, so here you can see the structure of the graphite, so these all are the covalent bonds and in between these the Van der Waals bonds are working on it, and this is the carbon atoms, so one layer by another layer there is only the Van der Waals bonds are working.



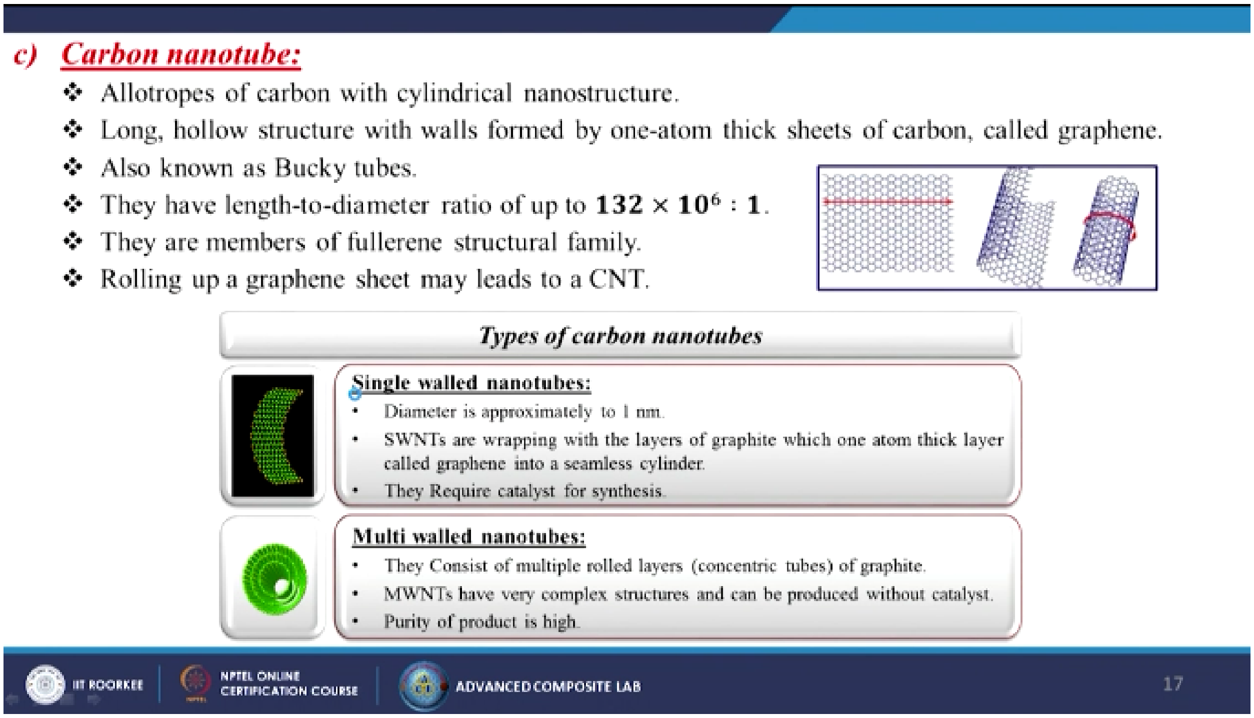
Properties of graphite:

- ❖ High strength and good chemical stability.
- ❖ High thermal conductivity.
- ❖ Low coefficient of thermal expansion.
- ❖ High resistance to thermal shock.
- ❖ High adsorption of gases and good machinability.

Uses of graphite:

- ➢ As heating element for electric furnaces.
- ➢ As electrodes for arc welding.
- ➢ In metallurgical crucibles.
- ➢ In casting molds for metal alloys and ceramics.
- ➢ For high temperature refractories etc.

What is the properties of graphite? Generally high strength and good chemical stability, high thermal conductivity, low coefficient of thermal expansions, high resistance to thermal shock, high adsorption of gases and the good machinability but they are so on. What is the use of graphite? As heating element for electric furnaces, as electrodes for arc welding in metallurgical crucibles, in casting molds for metal alloys and ceramics, for high temperature refractories etcetera.



c) *Carbon nanotube:*

- Allotropes of carbon with cylindrical nanostructure.
- Long, hollow structure with walls formed by one-atom thick sheets of carbon, called graphene.
- Also known as Bucky tubes.
- They have length-to-diameter ratio of up to $\mathbf{132 \times 10^6 : 1}$.
- They are members of fullerene structural family.
- Rolling up a graphene sheet may leads to a CNT.

Types of carbon nanotubes

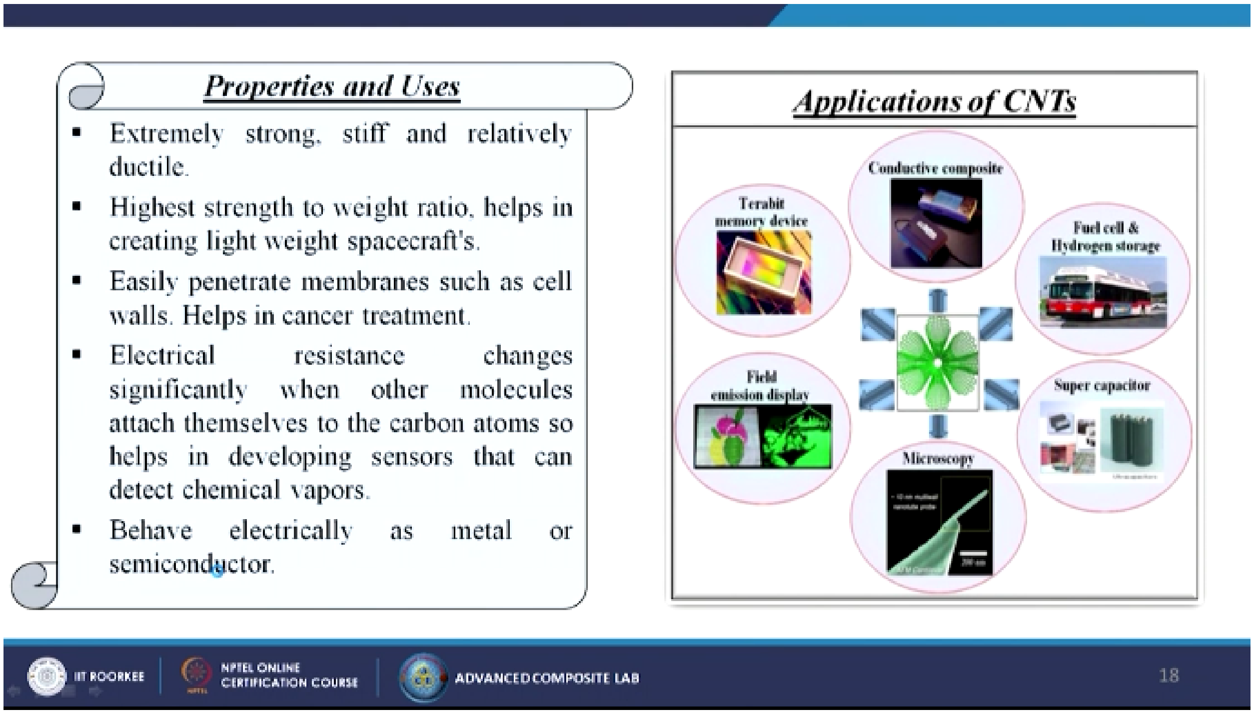
Single walled nanotubes:

- Diameter is approximately to 1 nm.
- SWNTs are wrapping with the layers of graphite which one atom thick layer called graphene into a seamless cylinder.
- They Require catalyst for synthesis.

Multi walled nanotubes:

- They Consist of multiple rolled layers (concentric tubes) of graphite.
- MWNTs have very complex structures and can be produced without catalyst.
- Purity of product is high.

So now we are going to discuss about the carbon nanotube, so allotropes of the carbon with cylindrical nanostructure, long hollow structure with walls formed by one-atom thick sheets of the carbon called the graphene, so simple graphene 2D in structure if we roll it generally we are thinking that is the carbon nanotube, also known as the Bucky tubes, they have length-to-diameter ratio of up to 132 x 10 to the power 6 is to 1, they are members of fullerene structural family, rolling up a graphene sheet may leads to a CNT, so they all are generally two types of carbon nanotubes, one is called the single walled carbon nanotubes, diameter is approximately to 1 nanometer, SWNT the short form of single walled nanotubes are wrapping with the layers of graphite which one atom thick layer called graphene into a seamless cylinder, they require catalyst for synthesis, so from this image you can better understand, and when we are talking about the multi walled carbon nanotubes, from the name itself you can understand that they are so many walls are present inside the carbon nanotubes, so here they consist of multiple rolled layers concentric tubes of the graphite, MWNT's have very complex structures and can be produced without catalyst, purity of product is high, from this image you can get the essence of the multi walled carbon nanotubes.



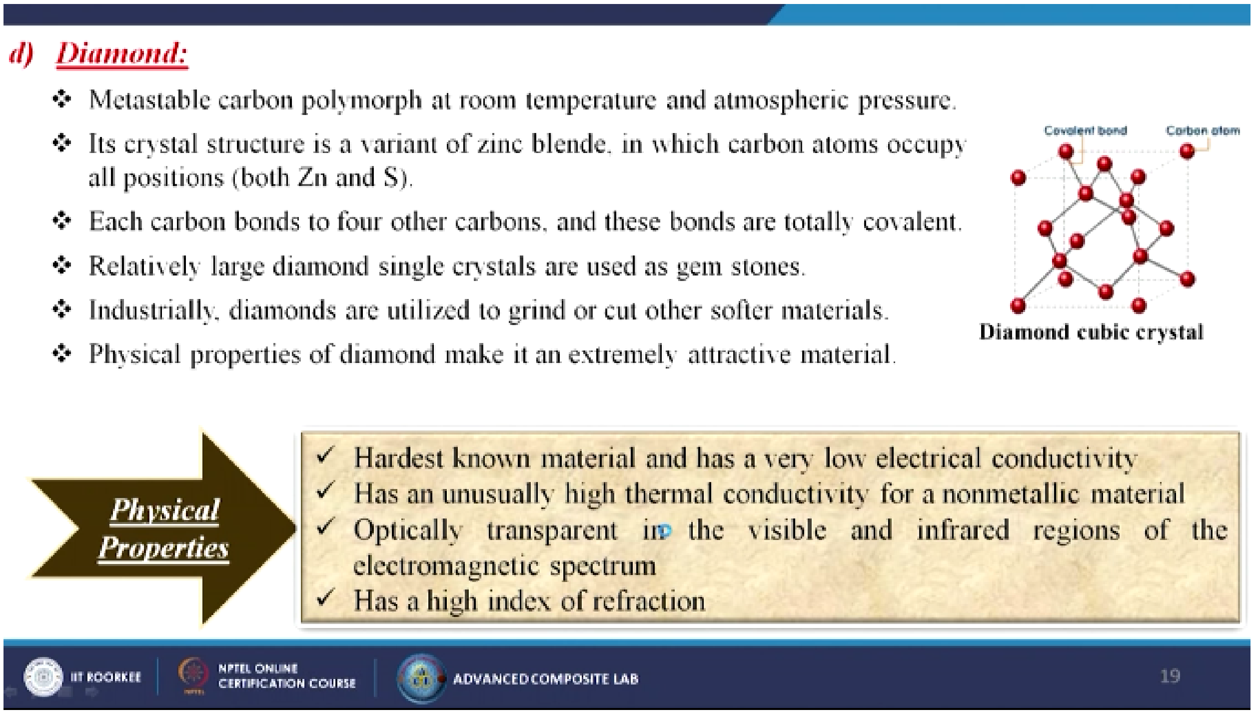
Properties and Uses

- Extremely strong, stiff and relatively ductile.
- Highest strength to weight ratio, helps in creating light weight spacecraft's.
- Easily penetrate membranes such as cell walls. Helps in cancer treatment.
- Electrical resistance changes significantly when other molecules attach themselves to the carbon atoms so helps in developing sensors that can detect chemical vapors.
- Behave electrically as metal or semiconductor.

Applications of CNTs

Now what are the properties and uses? Extremely strong, stiff and relatively ductile materials, high strength to weight ratio helps in creating the light weight spacecraft's, so generally for the aerospace applications or maybe high temperature applications, space shuttles we are using this carbon nanotubes easily penetrate membranes such as cell walls helps in cancer treatments, so that's why nowadays we are using it for the targeted drug delivery, electrical resistance changes significantly when other molecules attach themselves to the carbon atoms to help in developing sensors that can detect the chemical vapors, so that's why nowadays we are using it for the humidity sensors, biomolecule sensors, gas sensors and so on.

Next behave electrically as metal or maybe the semiconductor, so that's why we are using it for the energy storage or maybe energy generations, so what are the applications? It is, we are using for the memory device, high end memory device, we are using it for the conductive composites, fuel cell, hydrogen storage, super capacitor, microscopy, field emission display and the various so on.



d) Diamond:

- ❖ Metastable carbon polymorph at room temperature and atmospheric pressure.
- ❖ Its crystal structure is a variant of zinc blende, in which carbon atoms occupy all positions (both Zn and S).
- ❖ Each carbon bonds to four other carbons, and these bonds are totally covalent.
- ❖ Relatively large diamond single crystals are used as gem stones.
- ❖ Industrially, diamonds are utilized to grind or cut other softer materials.
- ❖ Physical properties of diamond make it an extremely attractive material.

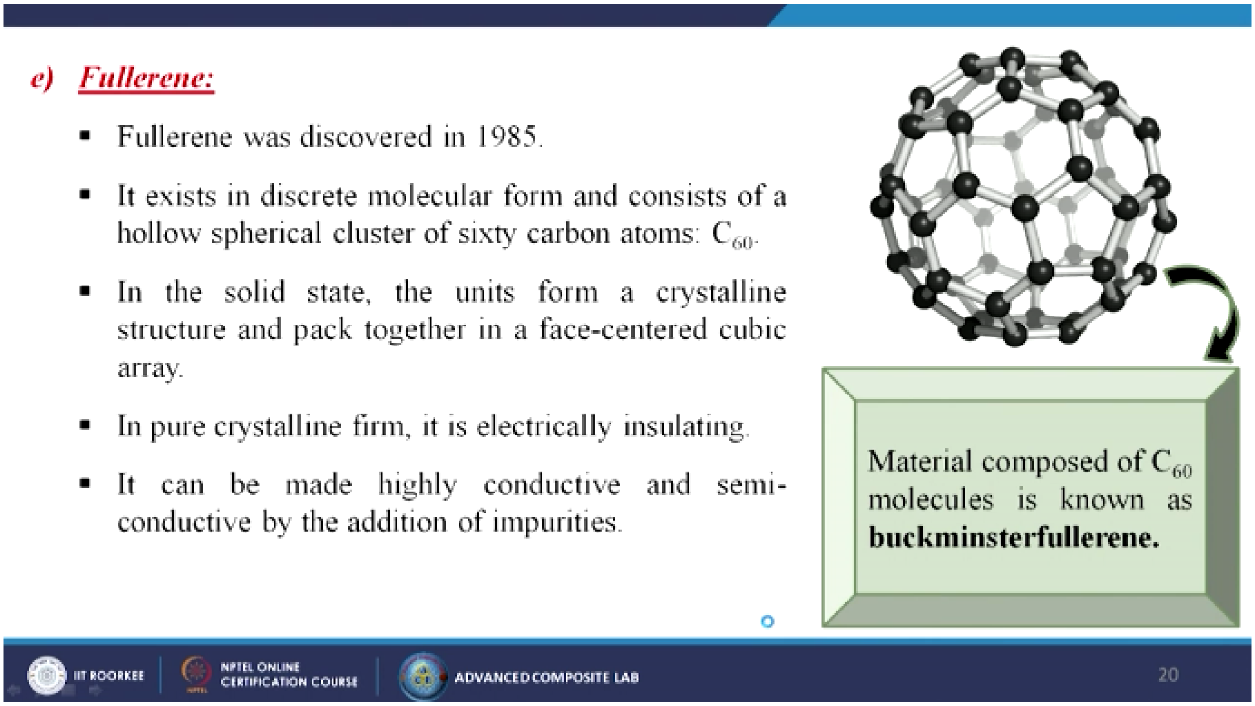
Diamond cubic crystal

Physical Properties

- ✓ Hardest known material and has a very low electrical conductivity
- ✓ Has an unusually high thermal conductivity for a nonmetallic material
- ✓ Optically transparent in the visible and infrared regions of the electromagnetic spectrum
- ✓ Has a high index of refraction

Now we are going to discuss about the diamond, so what is diamond? A metastable carbon polymorph at room temperature and atmospheric pressure, its crystal structure is a variant of zinc blende in which carbon atoms occupy the all positions, both zinc and the sulphur, each carbon bonds to four other carbons and these bonds are totally covalent bonds over there, so these all are the covalent bonds all.

Relatively large diamond single crystals are used as gem stones, generally we are using it as an ornament, industrially diamonds are utilized to grind or cut other softer materials, because it is the most hardest material till today, so that's why generally the artificial diamonds we are using it for cutting any kind of hard materials. Physical properties of diamond make it an extremely attractive material, what are the physical properties? Hardest known material and has a very low electrical conductivity this is number 1, then has an unusually high thermal conductivity for a nonmetallic material number 2, optically transparent in the visible and infrared regions of the electromagnetic spectrum that is number 3, and last has a high index of refraction that is number 4.

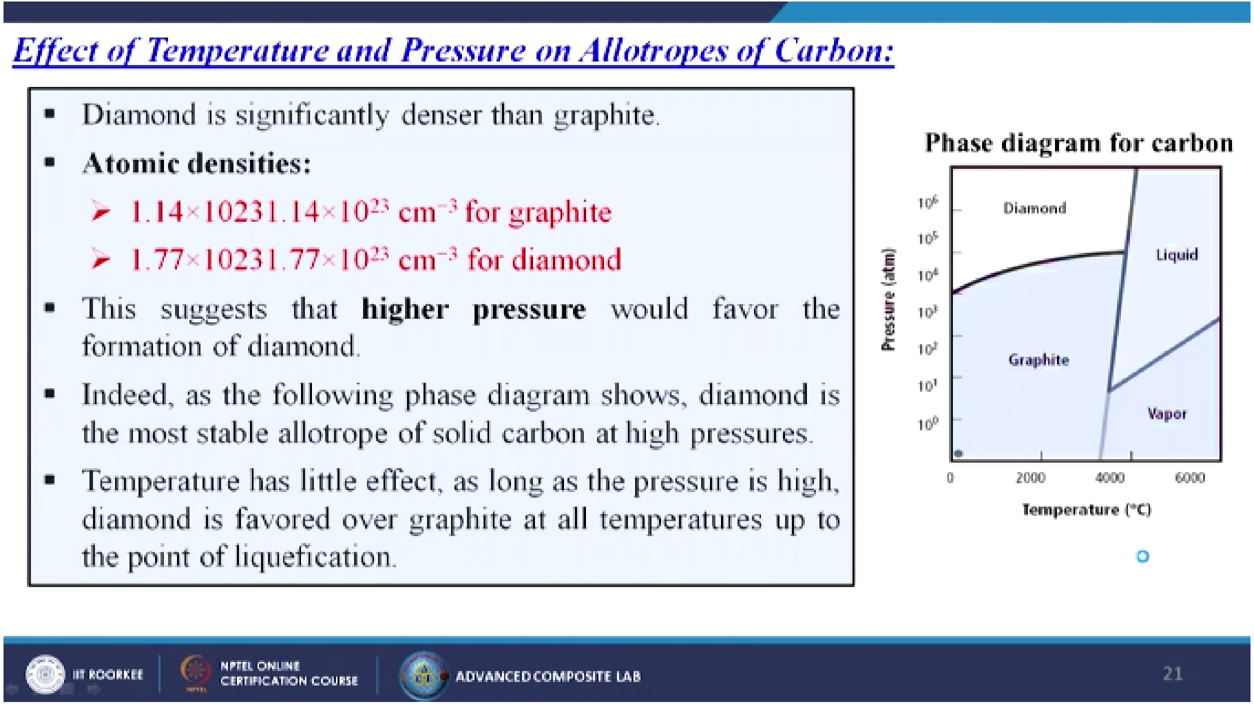


e) Fullerene:

- Fullerene was discovered in 1985.
- It exists in discrete molecular form and consists of a hollow spherical cluster of sixty carbon atoms: C_{60}.
- In the solid state, the units form a crystalline structure and pack together in a face-centered cubic array.
- In pure crystalline firm, it is electrically insulating.
- It can be made highly conductive and semi-conductive by the addition of impurities.

Material composed of C_{60} molecules is known as **buckminsterfullerene.**

Now we are going to discuss about the fullerene, so fullerene first it was discovered in the year of 1985, it exists in discrete molecular form and consists of a hollow spherical cluster of sixty carbon atoms, so that's why it is called the C60, so generally its looks like a football. In the solids state the units form a crystalline structure and pack together in a face centered cubic array, in pure crystalline form it is electrically insulating, it can be made highly conductive and semi-conductive by the additions of the impurities by doping, or maybe by some other means, so it the 360 structure molecule structure, it sometimes known as the buckminsterfullerene.



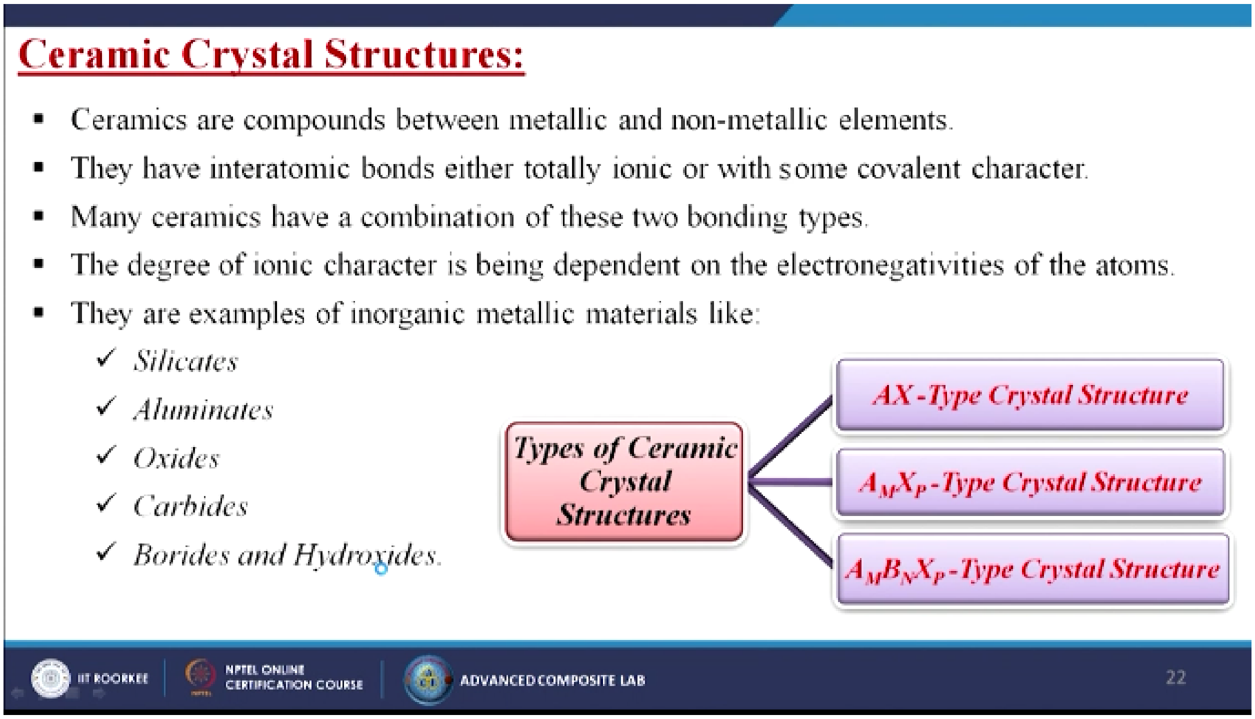
Effect of Temperature and Pressure on Allotropes of Carbon:

- Diamond is significantly denser than graphite.
- **Atomic densities:**
  - $1.14\times10231.14\times10^{23}$ cm^{-3} for graphite
  - $1.77\times10231.77\times10^{23}$ cm^{-3} for diamond
- This suggests that **higher pressure** would favor the formation of diamond.
- Indeed, as the following phase diagram shows, diamond is the most stable allotrope of solid carbon at high pressures.
- Temperature has little effect, as long as the pressure is high, diamond is favored over graphite at all temperatures up to the point of liquefication.

Phase diagram for carbon

Now we are going to discuss about the temperature and pressure effect on allotropes of carbon, so diamond is significantly denser than graphite, what is the atomic densities? So generally that 1.14 x 10231.14 x 10 to the power 23 per centimeter cube for graphite, and 1.77 x 10231.77 x 10 to the power 23 per centimeter cube for diamond, so atomic densities for the diamond is too high, this suggests that the higher pressure would favor the formation of diamond, so in this particular case if we see this one, this side the temperature is increasing and this side the pressure, atmospheric pressure is increasing, so diamond is at the top so that means for preparations of diamond you need a very high pressure, so it varies from generally 10 to the power 3 to more than that, then below that one is the graphite and if you increase the temperature so this is the vapor phase and this is the liquid phase.

Indeed, as the following phase diagram shows, diamond is the most stable allotrope of solid carbon at high pressure, temperature has little effect as long as the pressure is high diamond is favored over graphite at all temperatures up to the point of liquefications after that liquefication will start.

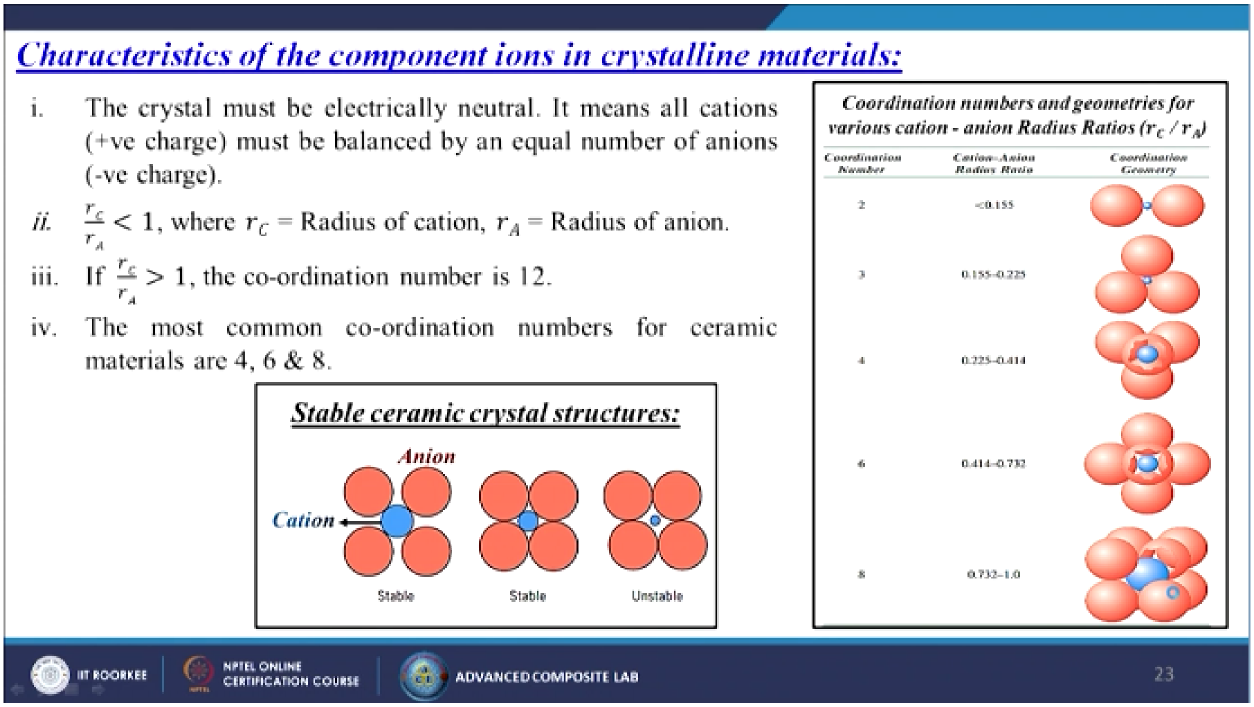


Ceramic Crystal Structures:

- Ceramics are compounds between metallic and non-metallic elements.
- They have interatomic bonds either totally ionic or with some covalent character.
- Many ceramics have a combination of these two bonding types.
- The degree of ionic character is being dependent on the electronegativities of the atoms.
- They are examples of inorganic metallic materials like:
  - ✓ *Silicates*
  - ✓ *Aluminates*
  - ✓ *Oxides*
  - ✓ *Carbides*
  - ✓ *Borides and Hydroxides.*

Types of Ceramic Crystal Structures
- *AX-Type Crystal Structure*
- *A_MX_P-Type Crystal Structure*
- *$A_MB_NX_P$-Type Crystal Structure*

Now we are going to discuss about the ceramic crystal structures, so ceramics are compounds between metallic and non-metallic elements that we have already gone through, they have interatomic bonds either totally ionic or with covalent characteristics, many ceramics have a combination of these two bonding types, so you can see ionic bond as well as you can see the covalent bond, that degree of ionic character is being dependent on the electronegativities of the atoms, they are examples of inorganic metallic materials like silicates, aluminates, oxides, carbides, borides and the hydroxides, so what are the ceramic crystal structure? Generally we can find AX-Type Crystal Structure, AM XP Type Crystal Structure, and the last one is that AM BN XP Type Crystal Structure.



Characteristics of the component ions in crystalline materials:

i. The crystal must be electrically neutral. It means all cations (+ve charge) must be balanced by an equal number of anions (-ve charge).

ii. $\frac{r_C}{r_A} < 1$, where r_C = Radius of cation, r_A = Radius of anion.

iii. If $\frac{r_C}{r_A} > 1$, the co-ordination number is 12.

iv. The most common co-ordination numbers for ceramic materials are 4, 6 & 8.

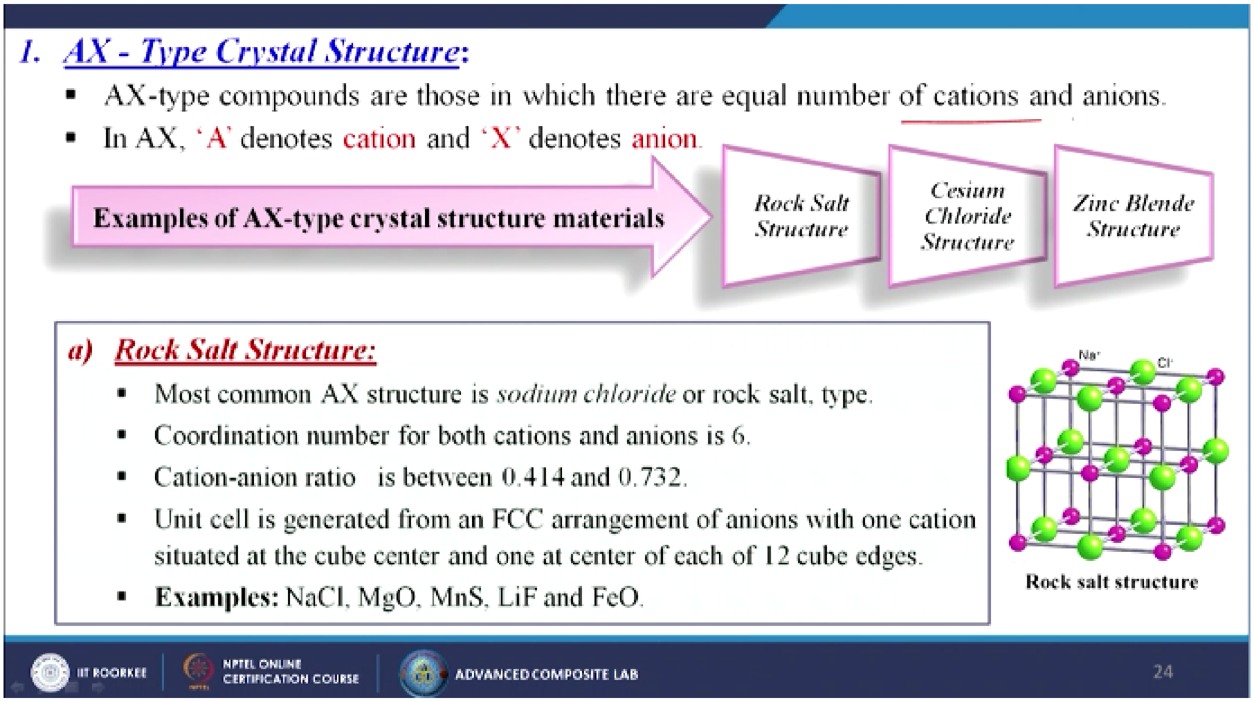
Stable ceramic crystal structures:

Coordination numbers and geometries for various cation - anion Radius Ratios (r_C / r_A)

Coordination Number	Cation–Anion Radius Ratio	Coordination Geometry
2	<0.155	
3	0.155–0.225	
4	0.225–0.414	
6	0.414–0.732	
8	0.732–1.0	

Now we are going to discuss one by one, so what is the characteristics of the component ions in crystalline materials? So the crystal must be electrically neutral, it means all cations positive charge must be balanced by an equal number of anions negative charge otherwise there will not be in the neutrality, so if RC/RA is less than 1, what is RC? RC is nothing but the radius of the cation, what is RA? RA is the radius of the anion, so RC/RA if it is less than 1, then third one will be if RC/RA greater than 1 the coordination number is 12, and the number 4 is that the most common coordination numbers for ceramic materials are 4, 6, and 8, so if you see in this particular case so coordination numbers and geometries for the various cation and anion radius factor RC/RA, so coordination number if it is 2 the cation anion radius ratio is less than is equal to 0.155, so you can see from this particular image, if we are talking about 4, so if we see the 4 it's varies from 0.225 to 0.414 and from this image you can get the picture, and then if we talk about the 8 so it is varies from 0.732 to 1, so what is the coordination geometry? The coordination geometry looks like this.

Now what is the stable ceramic crystal structures, so generally as I told already so it should be balanced, the cations and anions, so in this particular case this is the cations and it is surrounded by the four anions, it is stable, in this particular case also it is very very stable, but in this particular case it is under stable because there is some vacant positions in between that.



1. AX - Type Crystal Structure:

- AX-type compounds are those in which there are equal number of cations and anions.
- In AX, 'A' denotes cation and 'X' denotes anion.

Examples of AX-type crystal structure materials

Rock Salt Structure

Cesium Chloride Structure

Zinc Blende Structure

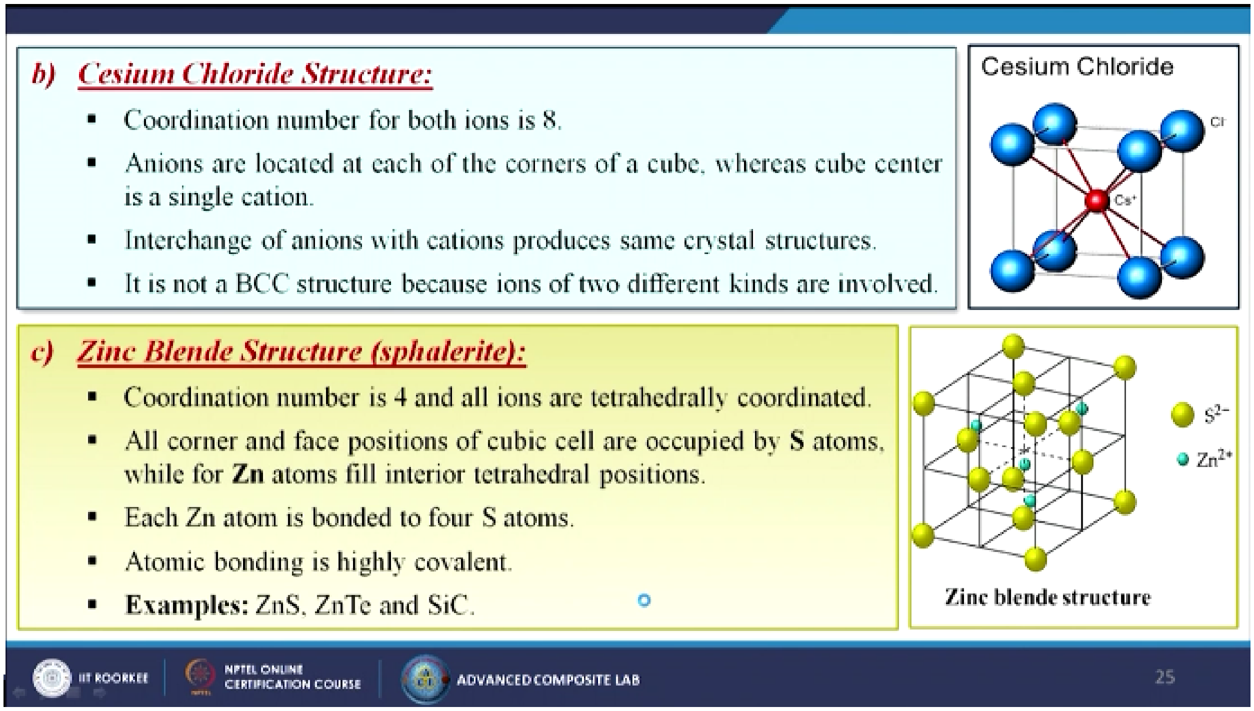
a) Rock Salt Structure:

- Most common AX structure is *sodium chloride* or rock salt, type.
- Coordination number for both cations and anions is 6.
- Cation-anion ratio is between 0.414 and 0.732.
- Unit cell is generated from an FCC arrangement of anions with one cation situated at the cube center and one at center of each of 12 cube edges.
- **Examples:** NaCl, MgO, MnS, LiF and FeO.

Rock salt structure

Now we are going to discuss about the AX-type crystal structure, so AX-type compounds are those in which they are equal number of cations and anions, this is the vital one so equal number of cations and anions. In AX, A denotes cations and X denotes anions, so example of AX-type crystal structure materials rock salt or maybe the sodium chloride, cesium chloride structures, zinc blende structures, so these all are the examples for AX-type crystal structure.

What is rock salt structure? Most common AX structure is sodium chloride or maybe the rock salt type, so coordination number for both cations and anion is 6, it is totally balanced, cation anion ratio is between 0.414 and 0.732, unit cell is generated from an FCC arrangement of anions with one cations situated at the cube center and one at center of each of 12 cube edges, so from this particular image you can understand that here chlorine is there, then after that here the chlorine is there, then after that two sides is the sodium then here it has been changed totally, then again it has been changed so it is, that's why it is called the AX-type crystal structure, so here all the cations and anions numbers are balanced, so what are the examples? Sodium chloride, magnesium oxide, manganese sulfide, lithium chloride, and the iron oxide.



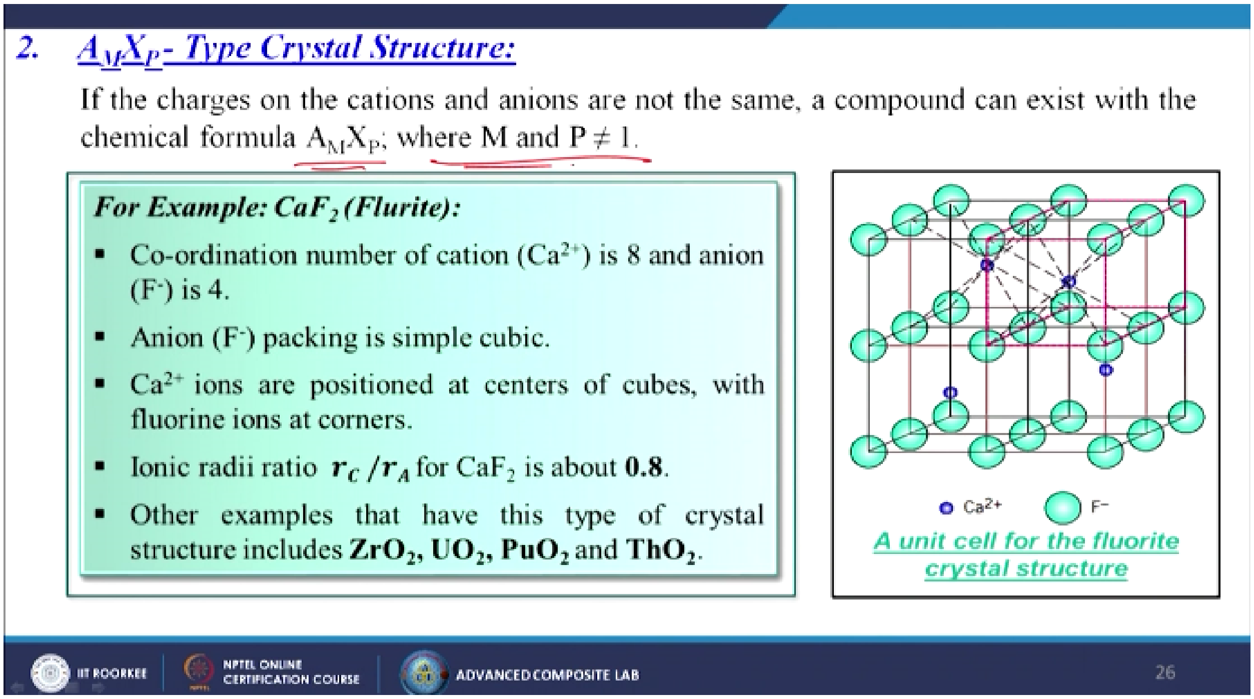
b) *Cesium Chloride Structure:*

- Coordination number for both ions is 8.
- Anions are located at each of the corners of a cube, whereas cube center is a single cation.
- Interchange of anions with cations produces same crystal structures.
- It is not a BCC structure because ions of two different kinds are involved.

c) *Zinc Blende Structure (sphalerite):*

- Coordination number is 4 and all ions are tetrahedrally coordinated.
- All corner and face positions of cubic cell are occupied by **S** atoms, while for **Zn** atoms fill interior tetrahedral positions.
- Each Zn atom is bonded to four S atoms.
- Atomic bonding is highly covalent.
- **Examples:** ZnS, ZnTe and SiC.

Now we can give the examples of the cesium chloride structure, so coordination number for both ions is 8, it’s balanced, anions are located at each of the corner of the cube here all are anions are present, and only in the cube center the cations is present. Interchange of anions with cations produces the same crystal structure, so if we change it, it is not a BCC structure because ions are two different kinds are involved, then we are going to discuss about the zinc blende structure or maybe in technical term we are calling it as a sphalerite, so coordination number is 4, and all ions are tetrahedrally coordinated, all corner and face positions of cubic cell are occupied by S atoms, while for zinc atoms fill interior tetrahedral positions, so this green in color are the zinc atoms and the yellow in color are the sulphur atoms. Each zinc atom is bonded to four sulphur atoms, atomic bonding is highly covalent, what is the examples? Zinc sulfide, zinc tellurium and silicon carbide.



2. A_MX_P- Type Crystal Structure:

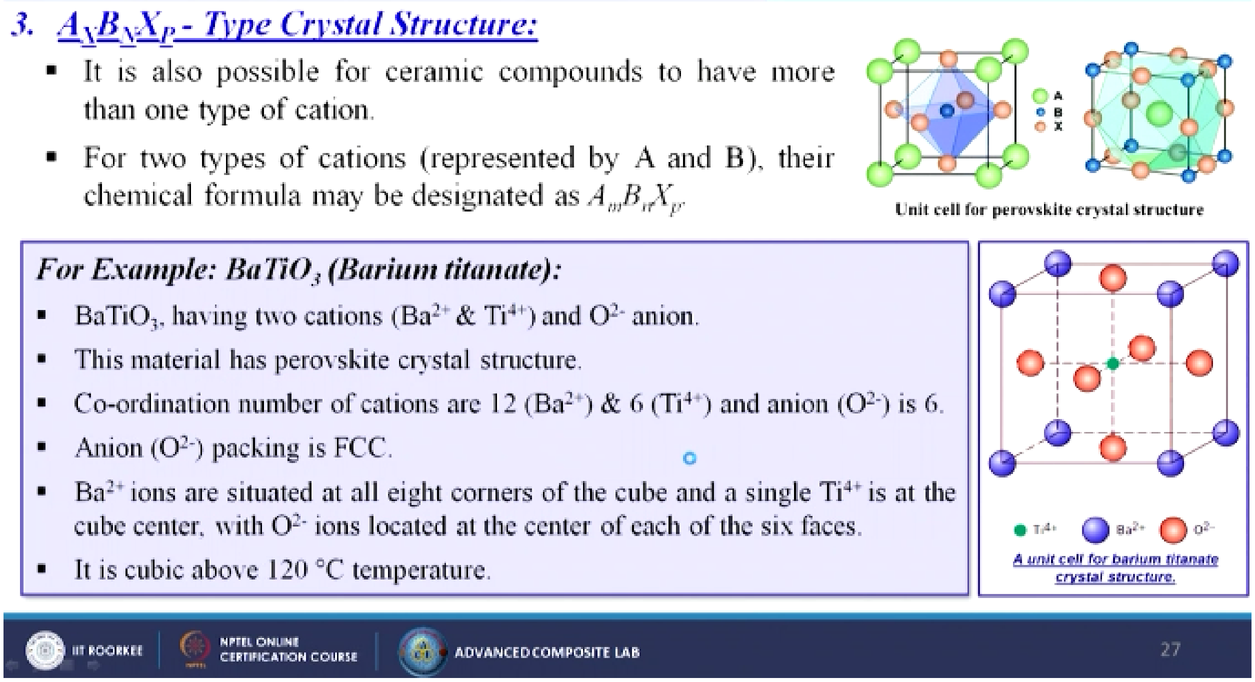
If the charges on the cations and anions are not the same, a compound can exist with the chemical formula A_MX_P; where M and P ≠ 1.

For Example: CaF_2 (Flurite):

- Co-ordination number of cation (Ca^{2+}) is 8 and anion (F^-) is 4.
- Anion (F^-) packing is simple cubic.
- Ca^{2+} ions are positioned at centers of cubes, with fluorine ions at corners.
- Ionic radii ratio r_C/r_A for CaF_2 is about **0.8**.
- Other examples that have this type of crystal structure includes **ZrO_2, UO_2, PuO_2** and **ThO_2**.

A unit cell for the fluorite crystal structure

Now we are going to discuss about the AM XP Type Crystal Structure, so if the charges on the cations and anions are not the same, a compound can exist with the chemical formula AM XP where M and P not is equal to 1, so for examples CAF2 which is known as the fluorite, coordination number of cation CA2+ is 8 and anion F- is 4, here it is not balanced, anion F- packing is simple cubic over here, so this blue in color all are the CA atoms and F are the, F- are maybe the fluorite anions, so calcium ions are positioned at centers of cubes with fluorine ions at corners, ionic radii ratio is RC/RA for calcium chloride CAF2 is about 0.8, other examples like zirconium oxide, uranium oxide, plutonium oxide or maybe the thorium oxides.



3. $A_XB_YX_P$- Type Crystal Structure:

- It is also possible for ceramic compounds to have more than one type of cation.
- For two types of cations (represented by A and B), their chemical formula may be designated as $A_mB_nX_p$.

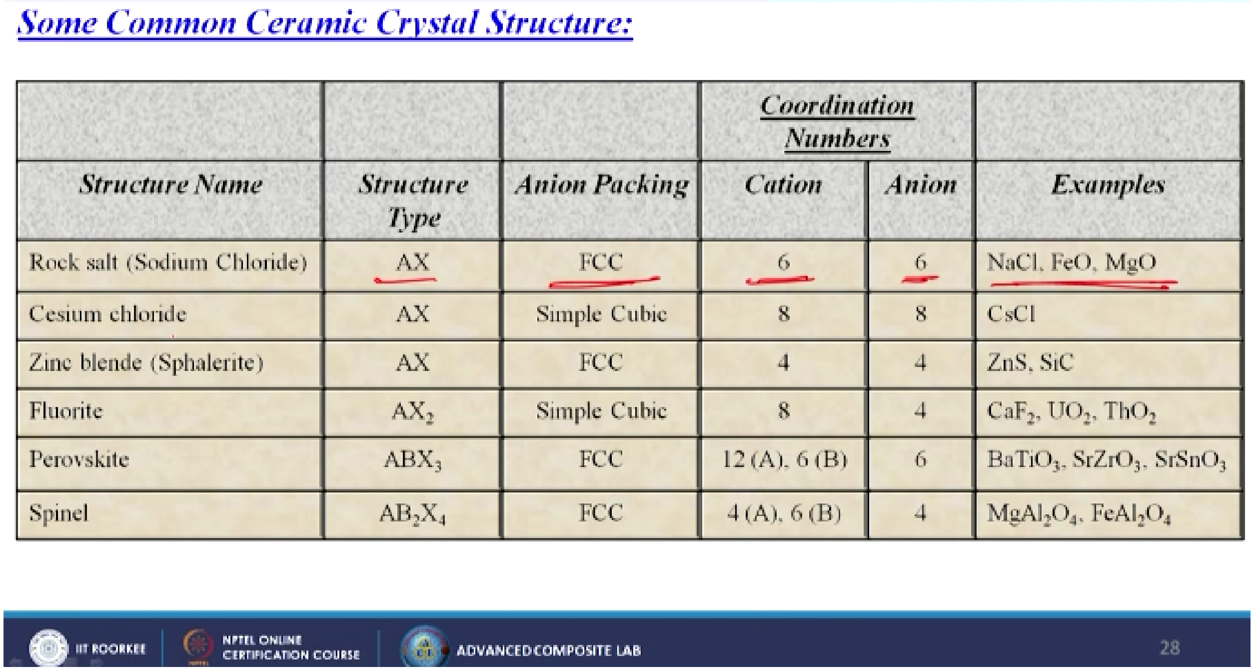
Unit cell for perovskite crystal structure

For Example: $BaTiO_3$ (Barium titanate):

- $BaTiO_3$, having two cations (Ba^{2+} & Ti^{4+}) and O^{2-} anion.
- This material has perovskite crystal structure.
- Co-ordination number of cations are 12 (Ba^{2+}) & 6 (Ti^{4+}) and anion (O^{2-}) is 6.
- Anion (O^{2-}) packing is FCC.
- Ba^{2+} ions are situated at all eight corners of the cube and a single Ti^{4+} is at the cube center, with O^{2-} ions located at the center of each of the six faces.
- It is cubic above 120 °C temperature.

A unit cell for barium titanate crystal structure.

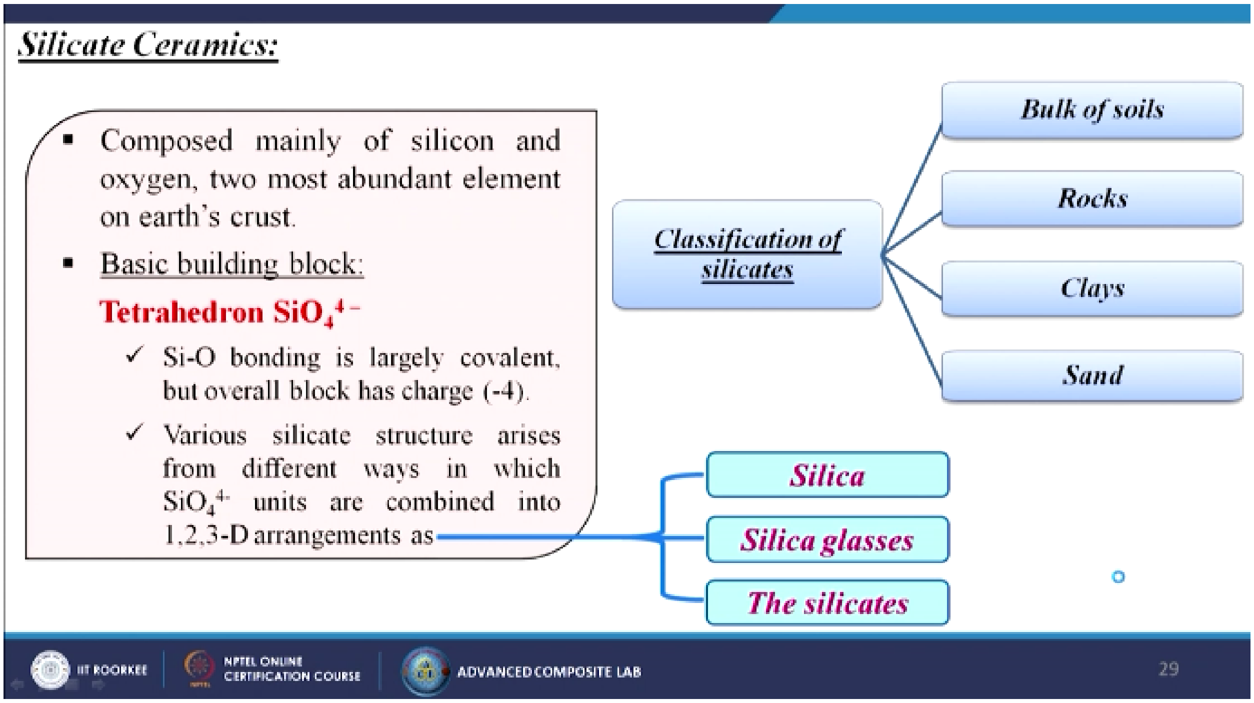
Now we are going to discuss about the AX BN XP Type Crystal Structure, so it is also possible for ceramic compounds to have more than one type of cations, so here generally two types of cations are present, so for two types of cations represented by A and B, their chemical formula maybe designated as AM BN XP, so for example BaTiO3 barium titanate, so in this particular case what happen? BaTiO3 having two cations Ba and Ti, so Ti is green in color and all the blue are the Ba and here O2- is acting as a anion over here, so anion O2- packing in FCC, Ba2+ ions are situated at all 8 corners of the cube and the single Ti4+ is at the cube center, you can see from this particular image with O2- ions located at the center of each of the six phases, it is cubic above 120 degree centigrade temperature.



Some Common Ceramic Crystal Structure:

			Coordination Numbers		
Structure Name	***Structure Type***	***Anion Packing***	***Cation***	***Anion***	***Examples***
Rock salt (Sodium Chloride)	AX	FCC	6	6	NaCl, FeO, MgO
Cesium chloride	AX	Simple Cubic	8	8	CsCl
Zinc blende (Sphalerite)	AX	FCC	4	4	ZnS, SiC
Fluorite	AX_2	Simple Cubic	8	4	CaF_2, UO_2, ThO_2
Perovskite	ABX_3	FCC	12 (A), 6 (B)	6	$BaTiO_3$, $SrZrO_3$, $SrSnO_3$
Spinel	AB_2X_4	FCC	4 (A), 6 (B)	4	$MgAl_2O_4$, $FeAl_2O_4$

So now some common ceramic crystal structure, examples so like rock salt structure type is AX at anion packing is FCC, here the cation number is 6, anion is 6, example sodium chloride FeO, MgO like that, cesium chloride so generally CsCl, so here it is simple cubic cation and anion number is also equal, for zinc blende also it is equal, zinc sulfide and silicon carbide, for fluorite generally it is AX2 type structure type, here the cation number is 8, and the anion number is 4, so CaF2 or UO2 or maybe ThO2, generally we are talking about the Perovskite materials nowadays it is been widely used for the solar cells, so generally the structure type is ABX3 or FCC in structure, so it is 12A and the 6B because 2 cations are present in this particular case, so anion is 6, like BiTiO3, SrZrO3, SrSnO3 like this, if we are talking about the spinel generally the crystal structure type is AB2X4, FCC in structure here also 2 cations are present 4A and 6B, and anions number are 4, so example is magnesium, aluminate, or maybe FeAl2O4.



Silicate Ceramics:

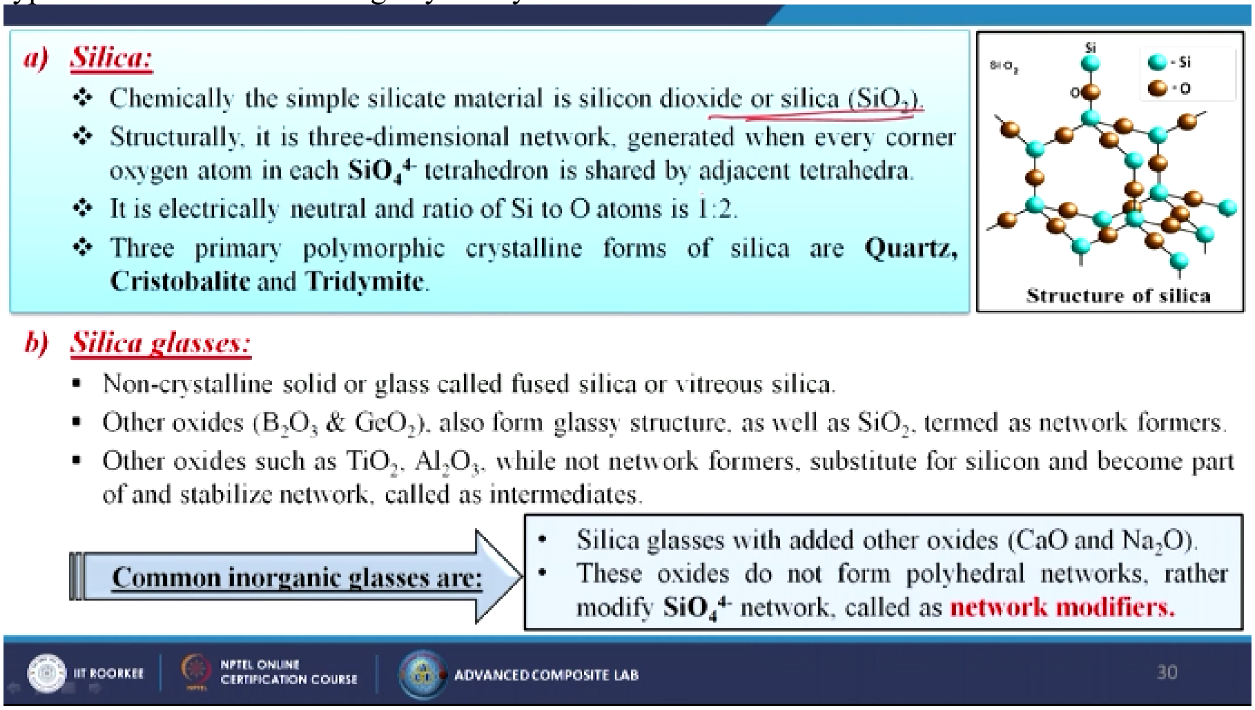
- Composed mainly of silicon and oxygen, two most abundant element on earth's crust.
- Basic building block:

  Tetrahedron SiO_4^{4-}

  - ✓ Si-O bonding is largely covalent, but overall block has charge (-4).
  - ✓ Various silicate structure arises from different ways in which SiO_4^{4-} units are combined into 1,2,3-D arrangements as
    - **Silica**
    - **Silica glasses**
    - **The silicates**

Classification of silicates
- **Bulk of soils**
- **Rocks**
- **Clays**
- **Sand**

Now we are going to discuss about the silicate ceramics, so generally it is composed mainly of silicon and oxygen, two most abundant element on earth's crust, so generally its having basic building block, so tetrahedron SiO4 4- so SiO bonding is largely covalent, but overall block has charge -4, various silicate structure arises from different ways in which SiO4 4- units are combined into 1, 2, 3D arrangement as silica, silica glasses, the silicates. So what is the classification of silicates? Generally bulk of soils, rocks, clays, and the sands, so generally this type of silicates we are seeing day to day life.



a) Silica:

- ❖ Chemically the simple silicate material is silicon dioxide or silica (SiO_2).
- ❖ Structurally, it is three-dimensional network, generated when every corner oxygen atom in each SiO_4^{4-} tetrahedron is shared by adjacent tetrahedra.
- ❖ It is electrically neutral and ratio of Si to O atoms is 1:2.
- ❖ Three primary polymorphic crystalline forms of silica are **Quartz, Cristobalite** and **Tridymite**.

Structure of silica

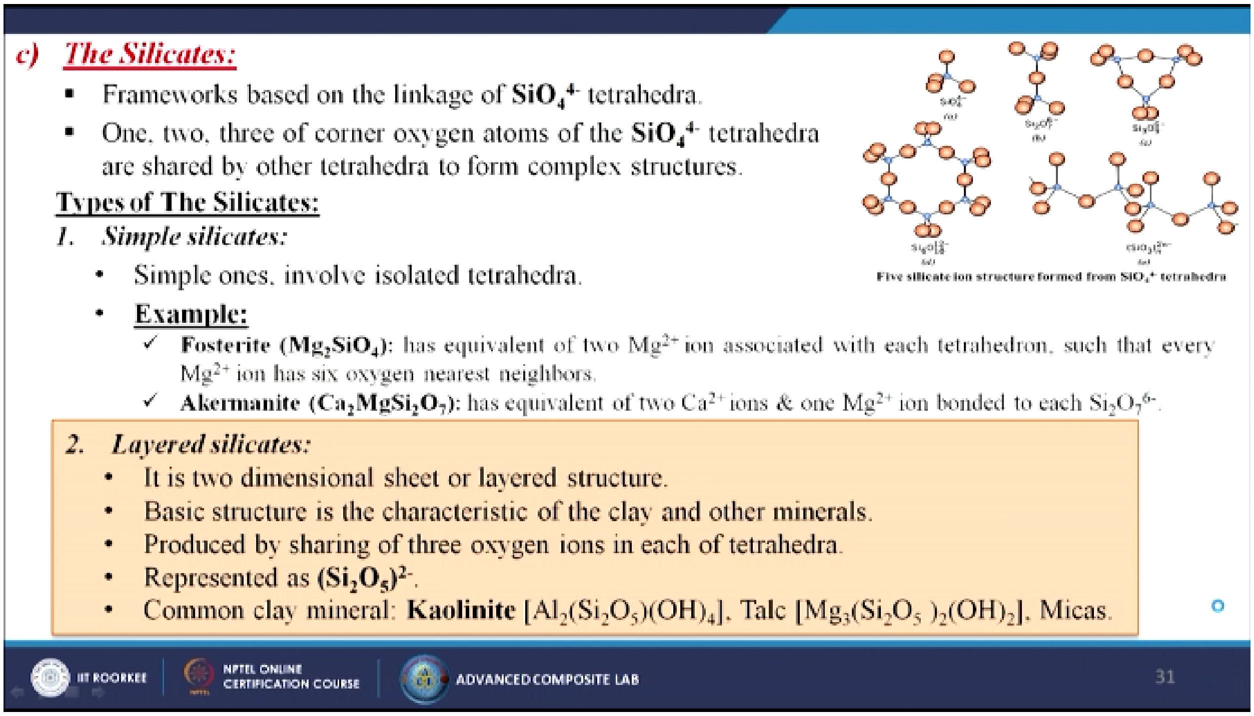
b) Silica glasses:

- Non-crystalline solid or glass called fused silica or vitreous silica.
- Other oxides (B_2O_3 & GeO_2), also form glassy structure, as well as SiO_2, termed as network formers.
- Other oxides such as TiO_2, Al_2O_3, while not network formers, substitute for silicon and become part of and stabilize network, called as intermediates.

Common inorganic glasses are:
- Silica glasses with added other oxides (CaO and Na_2O).
- These oxides do not form polyhedral networks, rather modify SiO_4^{4-} network, called as **network modifiers.**

What is silica? Chemically the simple silicate material is silicon dioxide or maybe the silica or SiO2, structurally it is three-dimensional network generated when every corner oxygen atom is each SiO4- tetrahedron is shared by the adjacent tetrahedron, so from this image you can see this one, it is electrically neutral and ratio of silicon to oxygen atom is 1:2, three primary polymorphic crystalline forms of silica generally we are seeing that is quartz, then cristobalite and the tridymite, Then another types is silica glasses, non-crystalline solid or glass called fused silica or maybe the vitreous silica, so other oxides like B2O3 and GeO2 germanium oxide also form glassy structure as well as SiO2 silicon dioxide terms at the network formers. Other oxides such as titanium dioxide TiO2 Al2O3 while not network formers substitute for silicon and become part of and stabilize network called as intermediates.

Common inorganic glasses are silica glasses with added other oxides like calcium oxide CaO or maybe the sodium oxide Na2O, this oxides do not form polyhedral network rather modify SiO4 4- network called as network modifiers.



c) *The Silicates:*

- Frameworks based on the linkage of $\mathbf{SiO_4^{4-}}$ tetrahedra.
- One, two, three of corner oxygen atoms of the $\mathbf{SiO_4^{4-}}$ tetrahedra are shared by other tetrahedra to form complex structures.

Types of The Silicates:

1. Simple silicates:

- Simple ones, involve isolated tetrahedra.
- **Example:**
  - ✓ **Fosterite ($\mathbf{Mg_2SiO_4}$):** has equivalent of two Mg^{2+} ion associated with each tetrahedron, such that every Mg^{2+} ion has six oxygen nearest neighbors.
  - ✓ **Akermanite ($\mathbf{Ca_2MgSi_2O_7}$):** has equivalent of two Ca^{2+} ions & one Mg^{2+} ion bonded to each $Si_2O_7^{6-}$.

2. Layered silicates:

- It is two dimensional sheet or layered structure.
- Basic structure is the characteristic of the clay and other minerals.
- Produced by sharing of three oxygen ions in each of tetrahedra.
- Represented as $\mathbf{(Si_2O_5)^{2-}}$.
- Common clay mineral: **Kaolinite** $[Al_2(Si_2O_5)(OH)_4]$, Talc $[Mg_3(Si_2O_5)_2(OH)_2]$, Micas.

Five silicate ion structure formed from SiO_4^{4-} tetrahedra

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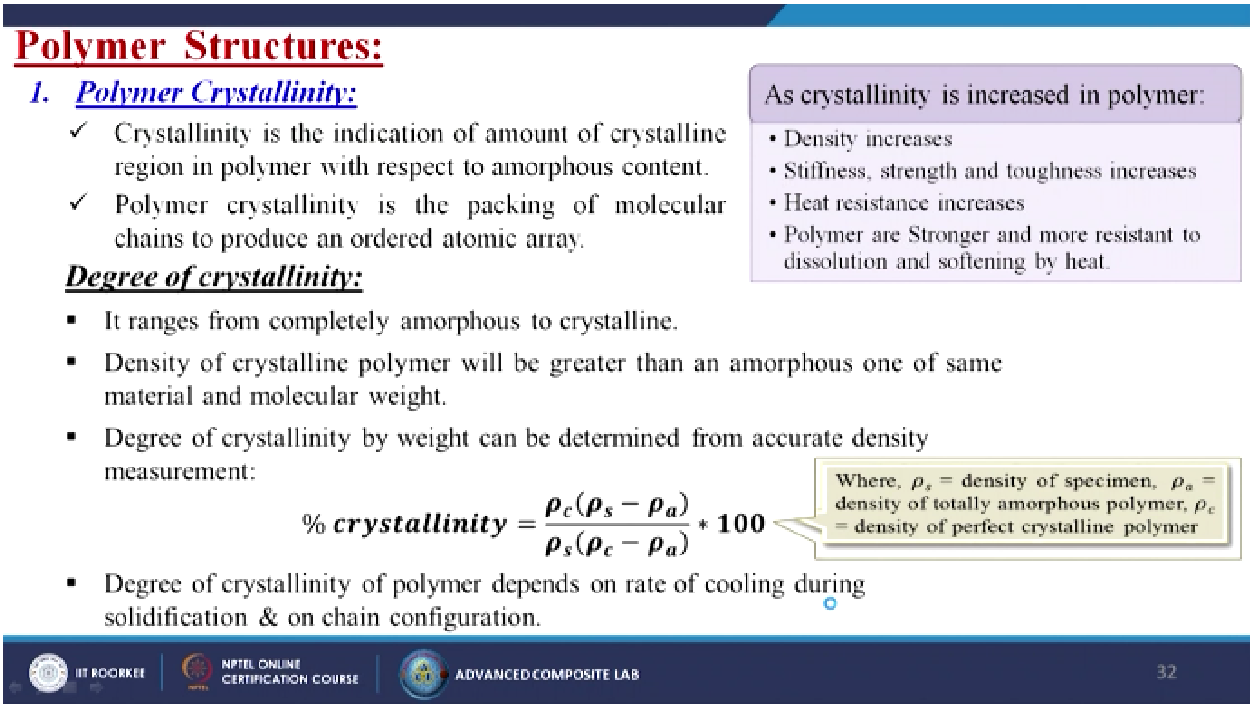
Then we are going to discuss about the silicates, so frameworks based on the linkage of SiO4 4- tetrahedra, one, two, three of corner oxygen atoms of the SiO4 4- tetrahedron are shared by other tetrahedra to form the complex structures.

Types of the silicates, simple silicates, simple ones involved isolated tetrahedra, what are the examples? So fosterite Mg2 SiO4 has equivalent of two Mg2+ ion associated with each tetrahedron such that every Mg2+ion has six oxygen nearest neighbors then akermanite Ca2MgSi2O7 has equivalent of two Ca2+ions and one Mg2+ion bonded to each Si2O7 6-.

What is layered silicate? It is two dimensional sheet or the layered structures from the name itself we can understand, basic structure is the characteristics of the clay and other minerals, produced by sharing of three oxygen atoms in each of the tetrahedra, represented as Si2O5 whole 2, common clay mineral kaolinite talc or maybe the mica.



Polymer Structures:

1. *Polymer Crystallinity:*

- ✓ Crystallinity is the indication of amount of crystalline region in polymer with respect to amorphous content.
- ✓ Polymer crystallinity is the packing of molecular chains to produce an ordered atomic array.

As crystallinity is increased in polymer:

- Density increases
- Stiffness, strength and toughness increases
- Heat resistance increases
- Polymer are Stronger and more resistant to dissolution and softening by heat.

Degree of crystallinity:

- It ranges from completely amorphous to crystalline.
- Density of crystalline polymer will be greater than an amorphous one of same material and molecular weight.
- Degree of crystallinity by weight can be determined from accurate density measurement:

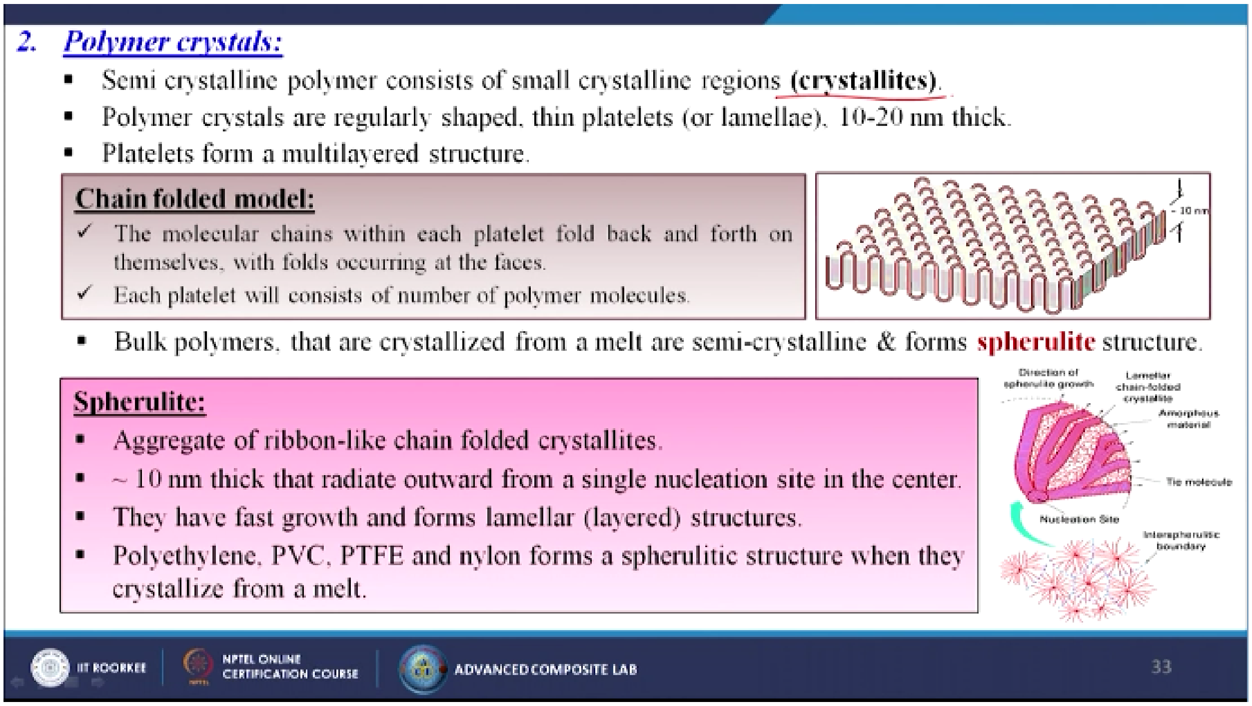
$$\% \, crystallinity = \frac{\rho_c(\rho_s - \rho_a)}{\rho_s(\rho_c - \rho_a)} * 100$$

Where, ρ_s = density of specimen, ρ_a = density of totally amorphous polymer, ρ_c = density of perfect crystalline polymer

- Degree of crystallinity of polymer depends on rate of cooling during solidification & on chain configuration.

Then we are going to discuss about the polymer structures, what about the polymer crystallinity? So crystallinity is the indication of amount of crystalline region in polymer with respect to amorphous content, polymer crystallinity is the packing of molecular chains to produce an ordered atomic array, as crystallinity is increased in polymer generally the density decreases, stiffness, strength, and toughness increases, heat resistance property increases, polymer are stronger and more resistance to dissolution and softening by the heat.

What is degree of crystallinity for the polymer? It ranges from completely amorphous to crystalline, density of crystalline polymer will be greater than an amorphous one of same material and molecular weight, degree of crystallinity by weight can be determined from accurate density measurement, what is that? Percentage crystallinity = rho C x rho S – rho A/rho S x rho C – rho A whole x 100 because we are calculating the percentage over there, where rho is the density of the specimen, rho is the density of total amorphous polymer, rho C is the density of perfect crystalline polymer, so generally degree of crystallinity of polymer depends on rate of cooling during solidifications and on chain configuration.



2. *Polymer crystals:*

- Semi crystalline polymer consists of small crystalline regions **(crystallites)**.
- Polymer crystals are regularly shaped, thin platelets (or lamellae), 10-20 nm thick.
- Platelets form a multilayered structure.

Chain folded model:

✓ The molecular chains within each platelet fold back and forth on themselves, with folds occurring at the faces.

✓ Each platelet will consists of number of polymer molecules.

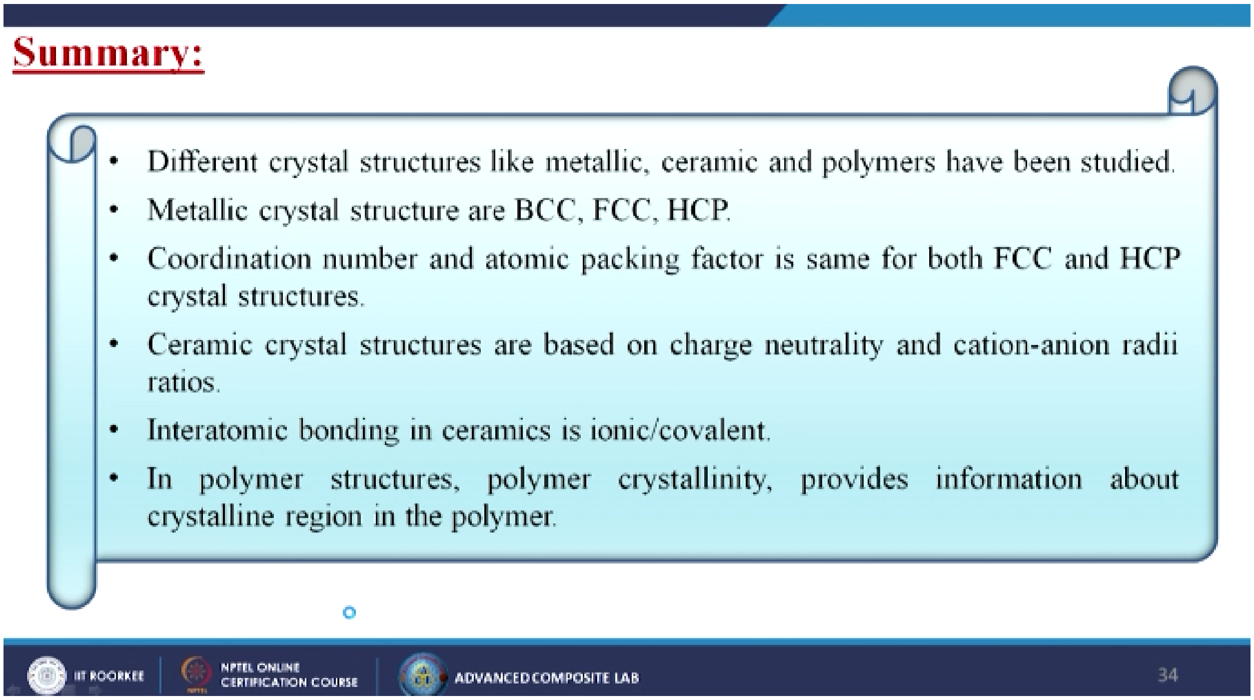
- Bulk polymers, that are crystallized from a melt are semi-crystalline & forms **spherulite** structure.

Spherulite:

- Aggregate of ribbon-like chain folded crystallites.
- ~ 10 nm thick that radiate outward from a single nucleation site in the center.
- They have fast growth and forms lamellar (layered) structures.
- Polyethylene, PVC, PTFE and nylon forms a spherulitic structure when they crystallize from a melt.

What is the polymer crystals? Semi crystalline polymer consists of small crystalline regions generally it is known as the crystallites, polymer crystals are regularly shaped, thin platelets or lamellae 10 to 20 nanometer thick, platelets form a multilayered structure, what is chain folded model? The molecular chains within each platelet fold back and forth on themselves with folds occurring at the faces itself, so you can see that it has been folded at the faces over there, each platelet will consist of number of polymer molecules, so generally the thickness is around 10 nanometer. Bulk polymers that are crystallized form a melt or semi crystalline and form the spherulite structure.

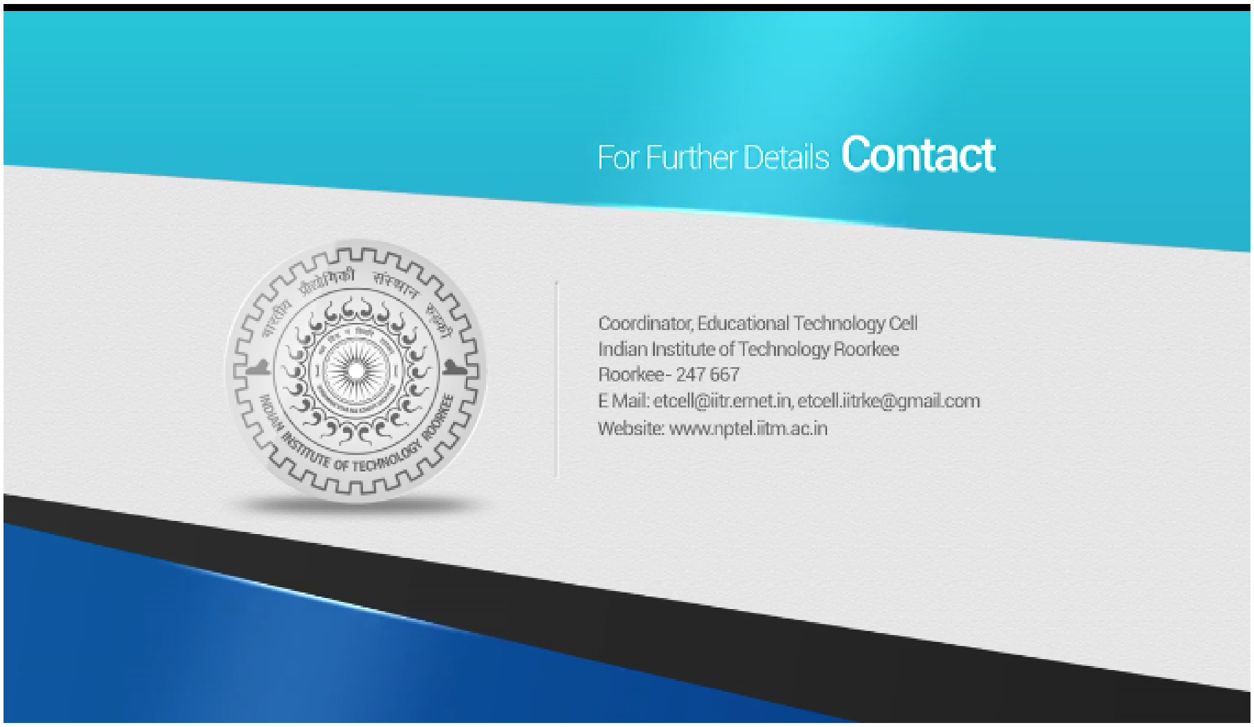
What is spherulite? Aggregate of ribbon like chain folded crystallites, so you can see from this particular image, so Inter-spherulitic boundary and these are all the spherulite structure. Generally 10 nanometer thick that radiate outward from a single nucleation site in the center, they have first growth and forms lamellar structures, polyethylene PVC, PTFE and nylon form a spherulitic structures when they crystallized from a melt.



Summary:

- Different crystal structures like metallic, ceramic and polymers have been studied.
- Metallic crystal structure are BCC, FCC, HCP.
- Coordination number and atomic packing factor is same for both FCC and HCP crystal structures.
- Ceramic crystal structures are based on charge neutrality and cation-anion radii ratios.
- Interatomic bonding in ceramics is ionic/covalent.
- In polymer structures, polymer crystallinity, provides information about crystalline region in the polymer.

Now we have come at to the last, so just we have to summarize the whole lecture, so in this particular lecture we have discussed about the different crystal structures like metallic, ceramic, and the polymers, then we have discussed about some metallic crystal structure thus like BCC, FCC, and the HCP, we have discussed about the coordination number and the atomic packing factor for the FCC and for the HCP crystal also. Ceramic crystal structures are based on charge neutrality and cation anion radii ratios that we have already discussed, we have discussed about the interatomic bonding in ceramics is ionic or maybe the covalent or maybe the both. In polymer structures, polymer crystallinity provides the information about crystalline region in the polymer itself. Thank you.



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