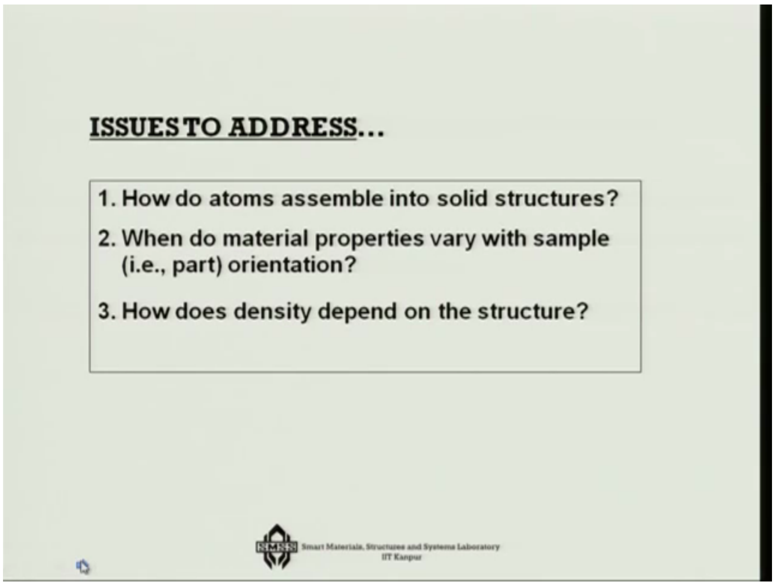
Nature and Properties of Materials
Professor Bishak Bhattacharya
Department of Mechanical Engineering
Indian Institute of Technology Kanpur
Lecture 8
The Role of Crystal Structure

Good morning, today we will talk about the role of Crystal structures. So we have already discussed about the material properties particularly the mechanical properties and the nature of atomic bonding. So now what we are going to focus on is actually how these atoms are assembled into a solid structure.

(Refer Slide Time: 00:43)



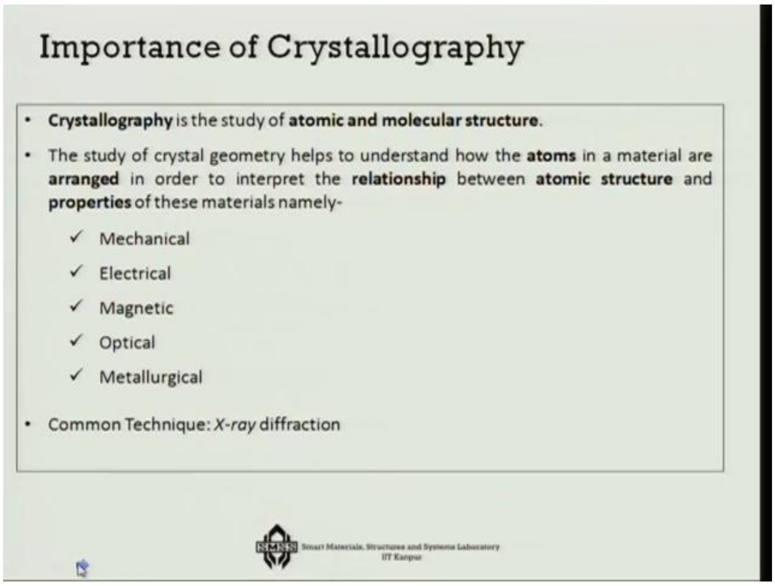
ISSUES TO ADDRESS...

1. How do atoms assemble into solid structures?
2. When do material properties vary with sample (i.e., part) orientation?
3. How does density depend on the structure?

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

And then what does it manifest in terms of the material properties because this material properties there are various types of structures which will generate different types of material properties. So how does for example, the density defend on the structure, as a case study we will see. So we will 1st of all look into the structure of the solid and then we will be material properties that get manifested from the solid.

(Refer Slide Time: 01:16)



Importance of Crystallography

- **Crystallography** is the study of **atomic and molecular structure**.
- The study of crystal geometry helps to understand how the **atoms** in a material are **arranged** in order to interpret the **relationship** between **atomic structure** and **properties** of these materials namely-
  - ✓ Mechanical
  - ✓ Electrical
  - ✓ Magnetic
  - ✓ Optical
  - ✓ Metallurgical
- Common Technique: *X-ray* diffraction

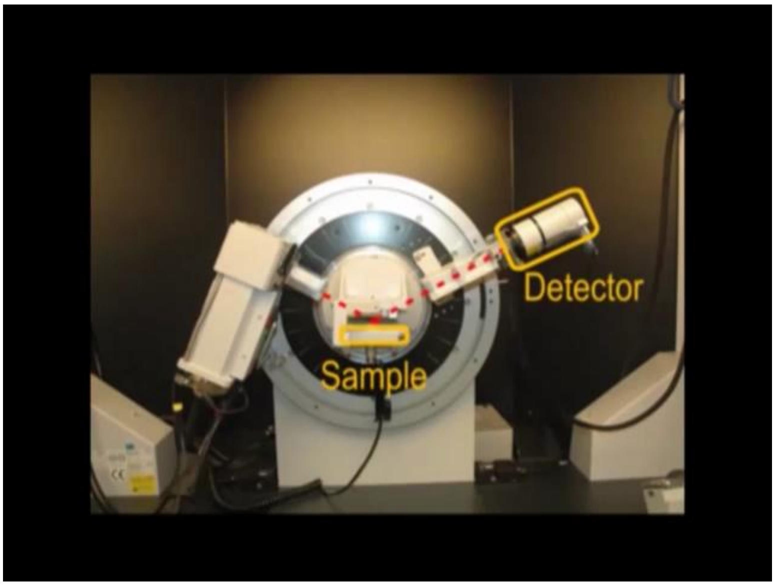
Smart Materials, Structures and Systems Laboratory
IIT Kanpur

Now here we will come to a very important topic which we have to know a little bit that is called the crystallography, which is nothing but the study of the atomic and molecular structure. The study of crystal geometric particularly because we will be working when on a ceramic materials and metals actually, which shows much more regular crystal structures.

This will help us to interpret the relationship between atomic structure and properties of these materials, properties for example, the mechanical properties, the electrical properties, magnetic, optical and metallurgical properties. Now all these things happen starting from somewhere around I would say 1867 to around 1915 or so.

The very basic development towards identifying the crystal structure of a material took place after the discovery of x-ray and the application of x-ray in terms of x-ray diffraction, which today very popularly is known as XR-D testing, so what is this XR-D testing actually? How to carry out x-ray diffraction test? So here I will try to explain in with the help of a beautiful video from the University of Washington, the Center on material and devices for information technology research.

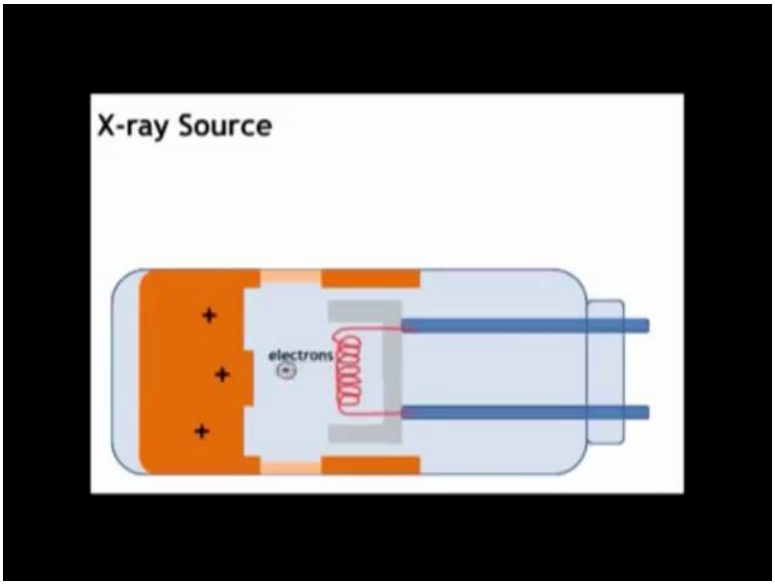
(Refer Slide Time: 2:55)



So let us look into this and then we will explain you that how you can carry out an x-ray diffraction testing. So as you can see here, this is actually a close up view of a x-ray diffraction testing machine of course, when the window of the machine is open because otherwise x-ray is very dangerous, so a very close up view.

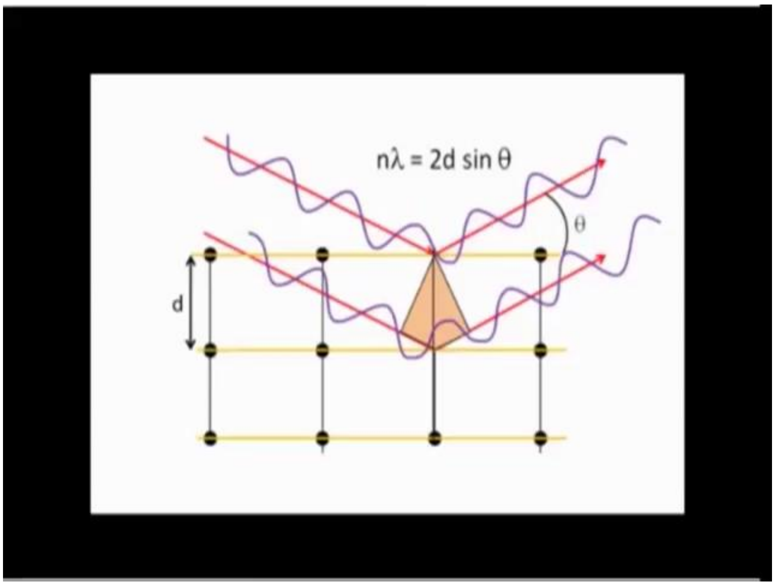
And as you can see that there are 3 important elements there. The left side, which is right now as you can see the left part of it, that is from where the incident x-ray is coming and the centre you have the sample and the right side you have the receiver, so that is what is the overall system. Now let us look into the video, which will give us some idea about how this system actually would work. To begin with, you must have a monochromatic x-ray source.

(Refer Slide Time: 03:53)


X-ray Source

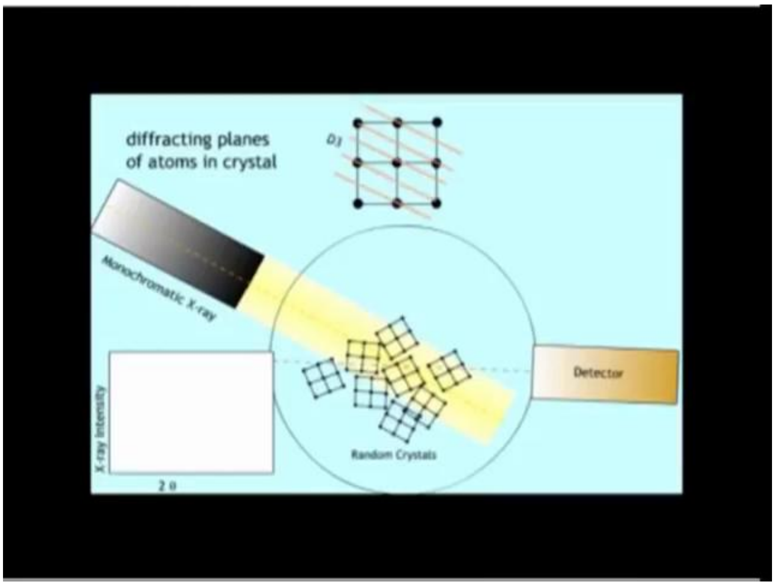
And in this case as you can see that the x-ray source is coming out of the system from a tungsten filament and it is going to a copper target and the x-ray passing through a Beryllium window is designed in such a manner that you get a monochromatic x-ray source.

(Refer Slide Time: 4:16)

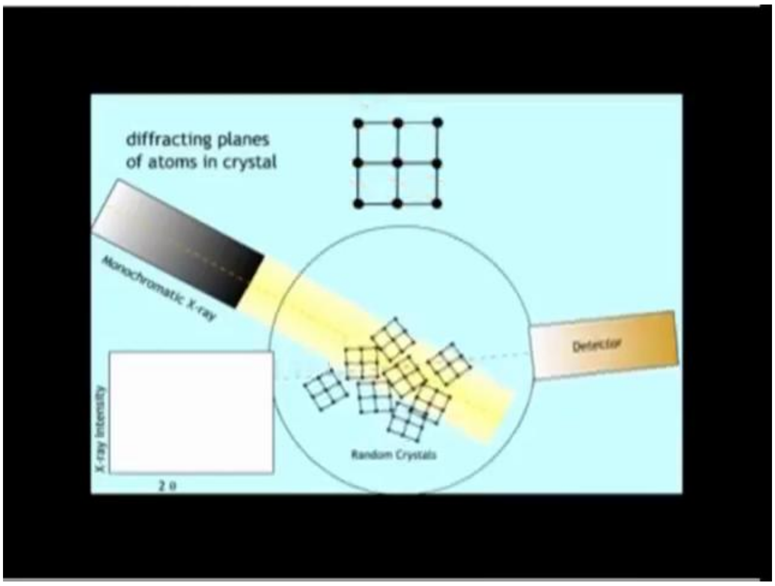


This monochromatic x-ray source is coming through the sample and from the sample it is going to the detector. Now, as you can see here that the wave is coming from the sample and from there it is going to the detector.

(Refer Slide Time: 04:27)



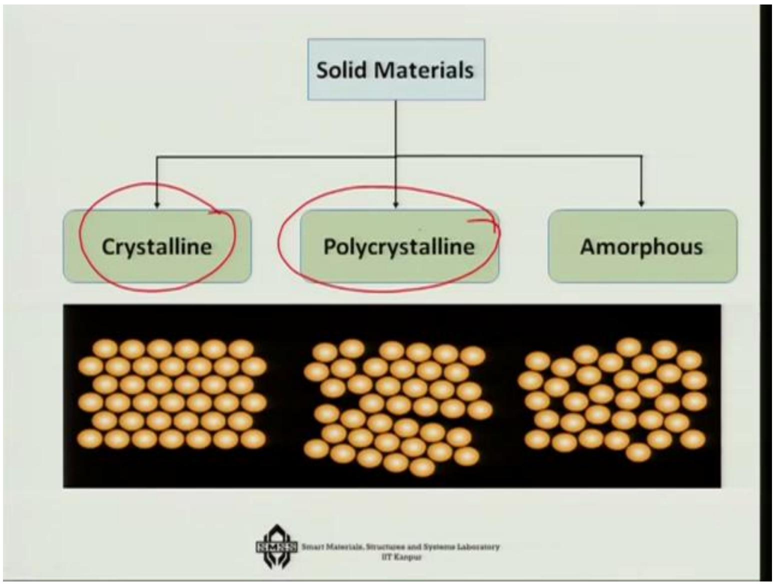
(Refer Slide Time: 04:29)



There is a certain ratio of the angle which is important in order to detect the crystal Lattice planes um. Basically, the whole thing works in such a manner as you are having regular crystal structure, the distance regular distance between this Lattice planes that works in terms of the diffraction of the crystals. So that actually generate what you call constructive interference in the system. And by looking at that constructive interference, we actually find out that what the kind of the crystal structure is if at all it has a crystal structure.

So thus every solid material can be subjected to this XR-D testing and we can find out that 1st information whether it is crystalline or not okay. If it is crystalline, there can be another variation that it may have actually many crystals, not a single crystal.

(Refer Slide Time: 05:39)


Solid Materials

Crystalline

Polycrystalline

Amorphous

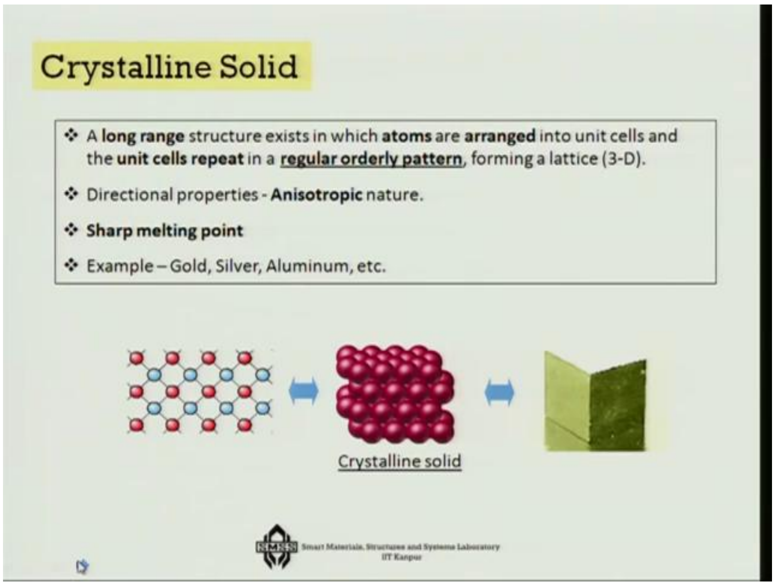
Smart Materials, Structures and Systems Laboratory
IIT Kanpur

So these are called the poly crystalline system. And there are some systems where you will not get regular order of Crystal Lattice and hence, these are actually amorphous systems for which you will not be able to observe the typical pictures that you will see corresponding to crystal Lattice structure in the crystalline or poly crystalline material, so these are called Amorphous structure.

So why we use x-ray to do this diffraction technique, it is because that the wavelength of the x-ray typically matches with the crystal plain separation distance, so it is between that 1 to 100 and strong kind of range. And hence x-ray can be used to resolve this picture and the brands it is a brand and it is further the people who got Noble prize in this direction.

And they are the 1st people who could actually make of course before that itself the XR-D was discovered, but they can make a connection between the two dimensional reflection that they are getting from these Crystal Lattices and the 3 dimensional structure of the crystal. So this actually later on revolutionized our understanding of the crystal structures, so that is what a little bit of history and genesis of x-ray diffraction, which is so important for determining whether a structure is crystalline or not.

(Refer Slide Time: 07:22)



Crystalline Solid

- A **long range** structure exists in which **atoms** are **arranged** into unit cells and the **unit cells repeat** in a **regular orderly pattern**, forming a lattice (3-D).
- Directional properties - **Anisotropic** nature.
- **Sharp melting point**
- Example – Gold, Silver, Aluminum, etc.

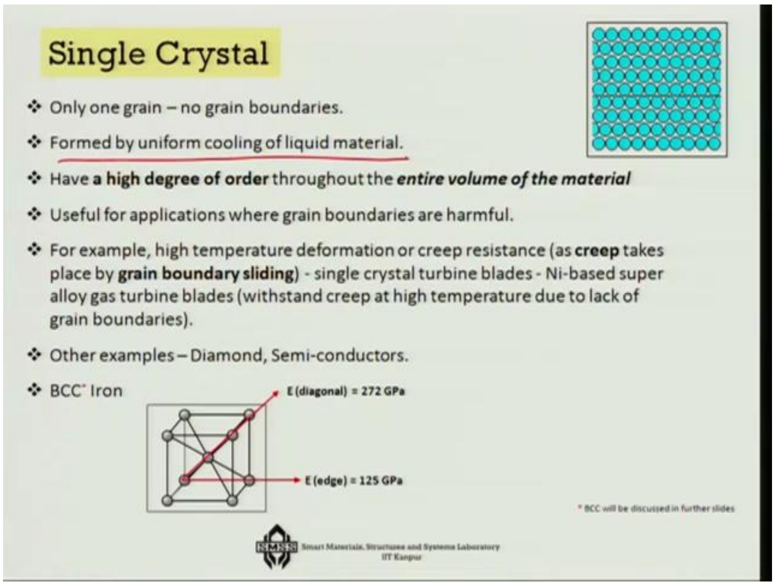
Smart Materials, Structures and Systems Laboratory
IIT Kanpur

Now formal definition, so crystalline solids how we call a solid to be crystalline? If you get a long length structure so that the atoms are arranged into unit cells and the unit cells repeat in a regular orderly pattern forming a 3 dimensional Lattice, then it will be a crystalline solid. And naturally, if they get arranged in a regular pattern then they will have actually directional properties like it will be anisotropic in nature.

Also, you will see that such systems will have a sharp melting and there are many examples of it for example, Gold, Silver, Aluminium many of the metals, they are the best examples of the crystalline solids. Now it is not only that it is only observing metals as I told you that many other structures which have ionic bond, they also show very good crystal structures.

And among the covalent bonds for example, Diamond also so very good crystal structure. So single, there are 2 types of I told you that a material can have a single crystal structure that means, it will have only one grain and that grain itself every grain we typically say as one crystal structure. So if there is a poly crystalline structure, then there are many grain boundaries around it.

(Refer Slide Time: 09:12)



Single Crystal

- Only one grain – no grain boundaries.
- Formed by uniform cooling of liquid material.
- Have a **high degree of order** throughout the ***entire volume of the material***
- Useful for applications where grain boundaries are harmful.
- For example, high temperature deformation or creep resistance (as **creep** takes place by **grain boundary sliding**) - single crystal turbine blades - Ni-based super alloy gas turbine blades (withstand creep at high temperature due to lack of grain boundaries).
- Other examples – Diamond, Semi-conductors.
- BCC* Iron

* BCC will be discussed in further slides

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

So only one grain, no grain boundaries and it is generally formed by a uniform cooling of liquid material, there are various techniques towards this and it will have a high degree of order throughout entire volume of the material. Development of a single crystal structure is quite an art on its own, but it has very practical applications. For example, one practical application is in terms of all these computer industries.

Because the silicon chips that are developed, if you make the silicon chips of poly crystals and structures, then the grain boundaries will act to the noise, so the microprocessor should not work properly. On the other hand, if you can make a single crystal structure in which the grain boundaries are absent, then this type of structures will be very good in terms of processing, et cetera, their processing time will be much faster.

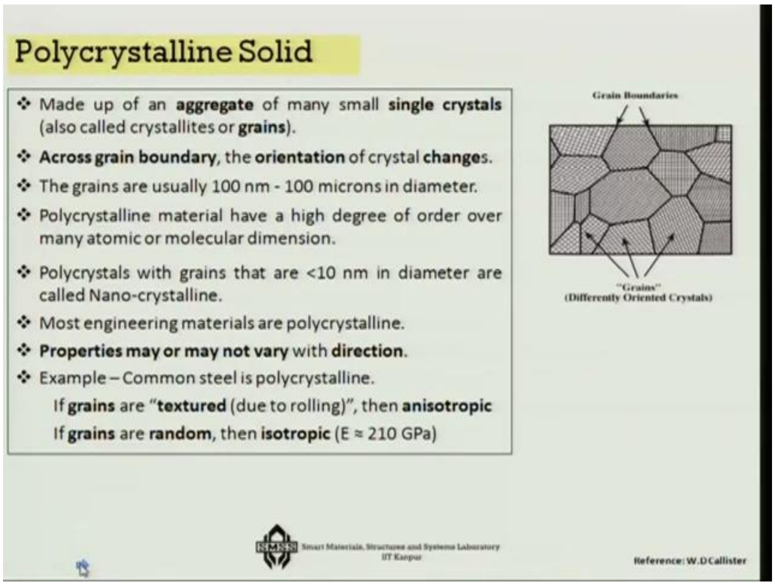
So it is one of the drive of the single crystal structure actually comes from the silicon industry itself, which actually manifests in terms of the computer industry. The other one is in terms of aircraft industry for example, I told you that creeping is a very crucial mechanical problem for turbine blades, which operates at a very high temperature and along with that at high stress level, so creeping is a very critical problem in such cases.

Now, creeping takes place by the grain boundary sliding okay. So if you can develop single crystal turbine blades for example, Ni-based super alloy gas turbine blade is a single crystal of Nickel or single crystal of titanium blades. These are actually very good in terms of creep's strength. So that is where another application of a single crystal structure is.

A typical example of a anisotropic of a single crystal structure, if you consider for example a BCC structure of iron, what is a BCC structure, we discuss about it very soon. You will see that along one edge it is about 125gigapascal as the modulus of elasticity, whereas along the diagonal it is about 272gigapascal. What it means is that the BCC structure of iron is extremely stiff along the diagonal direction.

Whereas, in anyone of the edges, it is actually much more flexible, so thus it will be if you develop now these single crystal iron structure, you will see a particular direction where actually it is very stiff, so that actually give the anisotropic property of a single crystal. Now let us come to the polycrystalline solid because this is actually much more practical because there are always impurities in a material.

(Refer Slide Time: 12:02)



Polycrystalline Solid

- Made up of an **aggregate** of many small **single crystals** (also called crystallites or **grains**).
- **Across grain boundary**, the **orientation** of crystal **changes**.
- The grains are usually 100 nm - 100 microns in diameter.
- Polycrystalline material have a high degree of order over many atomic or molecular dimension.
- Polycrystals with grains that are <10 nm in diameter are called Nano-crystalline.
- Most engineering materials are polycrystalline.
- **Properties may or may not vary** with **direction**.
- Example – Common steel is polycrystalline.
  If **grains** are "**textured** (due to rolling)", then **anisotropic**
  If **grains** are **random**, then **isotropic** (E ≈ 210 GPa)

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

Reference: W.D Callister

So they are basically as I have mentioned here that their aggregate of many small single crystals, they are also called crystallites or grains. So if there are grains, then they will be boundaries of the grains, which will be responsible for the deformation behavior, the stiffness and many other properties like the electrical property, the resistance, et cetera, everything depends on the grain structure and the grain boundary.

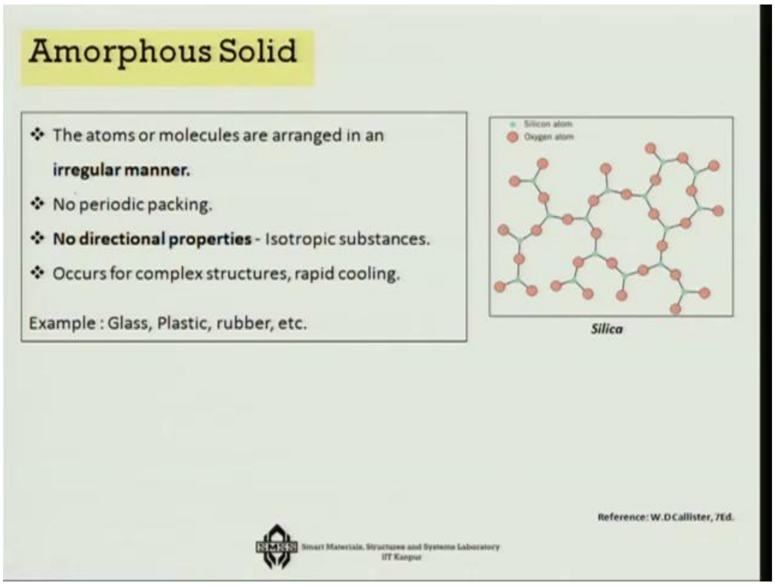
Now, it is the grain boundary where the orientation of the crystal will be changing because we will be having another crystal formation, so thus the orientation will be changing. These grains are generally in the range of 100 nanometre to 100 microns, naturally the larger the grain structure, the stiffer will be the structure, but it will be more anisotropic.

Now polycrystalline materials have high degree of order over many atomic or molecular dimensions, so they less than 10nanometre, if they are in diameter they are actually known as the nano crystalline materials. So they can be nano crystalline or microcrystalline or even at the micro range. Now, most of the engineering materials are actually poly crystalline in nature and their properties may or may not vary with the direction.

Why? Because the crystals that are indeed going to give anisotropic, so a single crystal or which is inside the grain will give you anisotropic. But since there are many grains and hence there are random distributions of anisotropic property, so this kind of gets averaged out and it can give you if there is no grain or direction kind of a orientation in the grain direction, it may give you anisotropic property.

So as an example common steel is actually poly crystalline and if the grains of this poly crystalline material are textured due to rolling, then it will become anisotropic okay. But if it is, the grains are random, and then it will be isotropic. So this also tells us about the significance of the manufacturing process that it will be subjected to. So thus a poly crystalline solid may or may not show isotropy depending on the manufacturing process.

(Refer Slide Time: 14:45)



Amorphous Solid

- The atoms or molecules are arranged in an **irregular manner.**
- No periodic packing.
- **No directional properties** - Isotropic substances.
- Occurs for complex structures, rapid cooling.

Example : Glass, Plastic, rubber, etc.

Silica

Reference: W.D Callister, 7Ed.

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

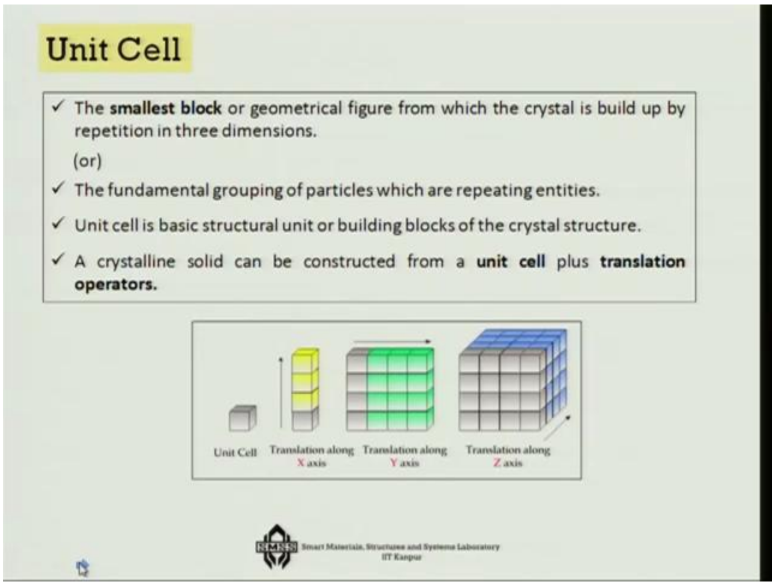
Now we have talked about single crystal and the polycrystalline, so naturally the last in the line is where you will not get a long-range order at all that mean the atoms and molecules are arranged in an irregular manner. So you will not get any periodic packing in such a system, you will not see any directional property in such a system; they are basically isotropic because of this reason.

And this can occur due to 2 reasons, one is that as I told you that the cooling process actually governs that whether you get enough time for the liquid to change to solid ways such that the regular the Lattice formation is possible. So with a very low cooling rate, you can even make metals as the glass and we call them to be Metglas okay. So I will talk about different types of metallic glasses okay.

Or something like BMG, bulk metallic glasses, they are becoming very important in today's context. So this is one may by controlling the cooling rate if it is the cooling rate is actually very slow, you get crystalline structure, but if you make the cooling rate to be very fast, then you get the glassy structure out of it, so that is one way of generating this offer structure.

Of course, the other things are at a later stage we will talk about it that is the polymeric chain. The polymers are by nature they are amorphous in nature because depending on what are coming in the cross chains of a polymer, it may never actually show a long range order. So there are some materials which are by nature amorphous and there are some materials which are by nature crystal, but you can force it to take an amorphous structure for example, this Bulk Metallic Glass or the metallic glasses.

(Refer Slide Time: 16:40)



Unit Cell

- ✓ The **smallest block** or geometrical figure from which the crystal is build up by repetition in three dimensions.

  (or)
- ✓ The fundamental grouping of particles which are repeating entities.
- ✓ Unit cell is basic structural unit or building blocks of the crystal structure.
- ✓ A crystalline solid can be constructed from a **unit cell** plus **translation operators.**

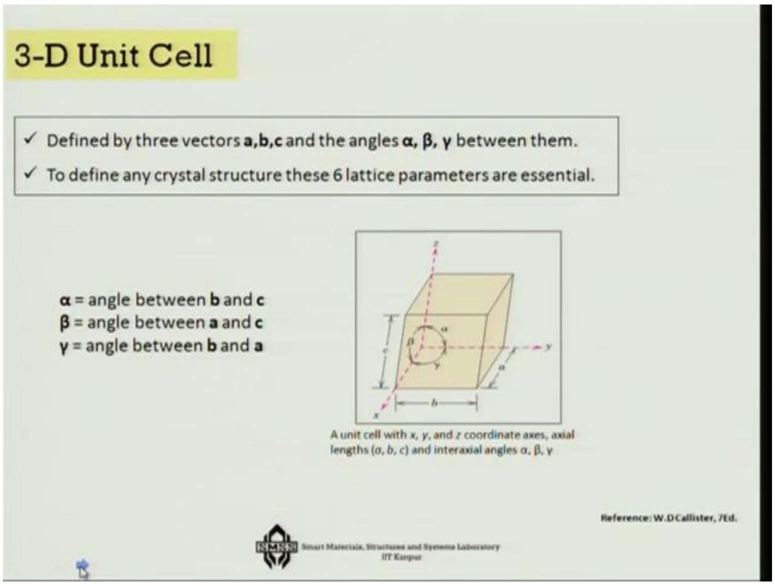
Smart Materials, Structures and Systems Laboratory
IIT Kanpur

Now, let us 1st concentrate on the structures which has regularity or a regular crystal structure. So the way to look at it is to look at something which is known as the unit cell okay, which is the smallest block or geometrical figure from which the crystal can be thought of that it is build up by repetition in the 3 dimension.

So this unit cell or so to say the basic structure unit or the building block of the crystal structure, it can be constructed basically a crystalline solid can be constructed from unit cell along with a translational operator for example, you can see that this is a unit cell. Suppose a cubic unit cell and if it has translation only around one direction, you get a particular type of structure.

If it has translation in 2 directions, you get this type of a structure, if it has translation on all the 3 directions; you get this kind of a Rubik cube structure. So thus, unit cell with a translational operator will actually develop the complete solid structure.

(Refer Slide Time: 17:48)



3-D Unit Cell

- ✓ Defined by three vectors **a,b,c** and the angles **α, β, γ** between them.
- ✓ To define any crystal structure these 6 lattice parameters are essential.

α = angle between **b** and **c**
β = angle between **a** and **c**
γ = angle between **b** and **a**

A unit cell with x, y, and z coordinate axes, axial lengths (a, b, c) and interaxial angles α, β, γ

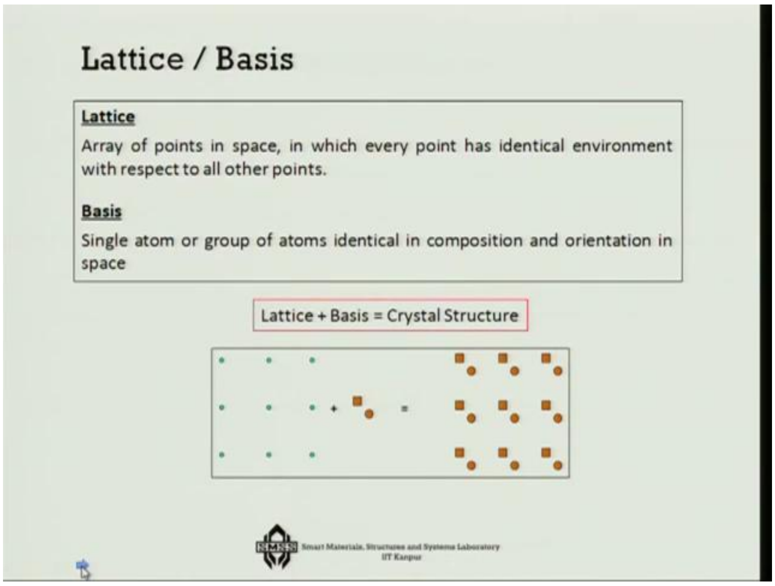
Reference: W.D Callister, 7Ed.

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

Now, in a 3D unit cell, how do we define the unit cell? There are 6 parameters to define a unit cell, okay. So these 6 parameters are what, there are 3 vectors a, b, c as you can see. Each one of these vectors a, b and c are to the 3 directions okay so x, y, z and these directions need not be perpendicular to each other, okay. So these are the edges, along the edges of the crystal Lattice.

Only in a very special case, in some of the special cases the angle between them will be 90 degree otherwise, we can assume them to be as generic like Alpha, Beta and Gamma. So Alpha, if you consider from any angle between b and c by definition, Beta is angle between a and c, and Gamma is the angle between b and a, so this is what is the 3 angles; Alpha, Beta and Gamma and this a, b, c, they define a generic 3D unit cell.

(Refer Slide Time: 18:57)



Lattice / Basis

Lattice

Array of points in space, in which every point has identical environment with respect to all other points.

Basis

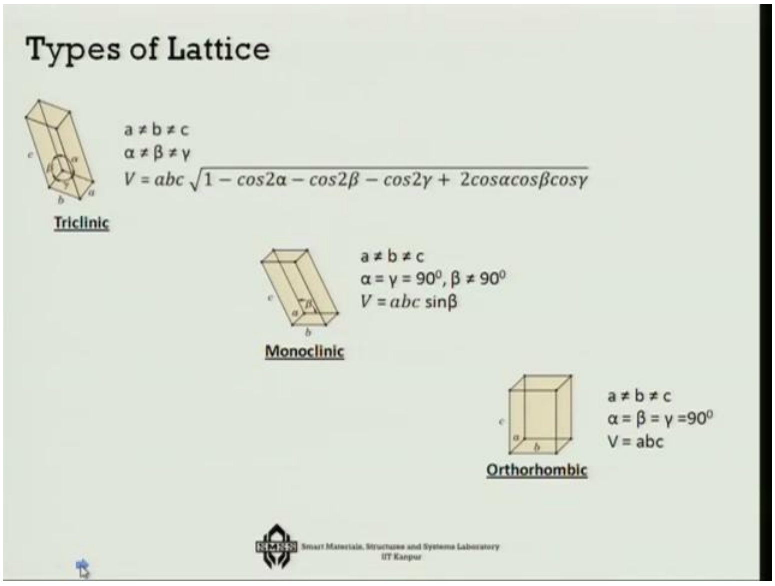
Single atom or group of atoms identical in composition and orientation in space

Lattice + Basis = Crystal Structure

Now from there one more point we have to keep in our mind that there are 2 important things here, one is called the Lattice and another is called the Basis. What is a Lattice? It is an array of points in space, in which every point has identical environment with respect to all other points okay. For example, this is a Lattice structure where every point has an identical environment with respect to the other points.

And the Basis is actually the single atom okay or a group of items identical in composition and orientation in space. So a crystal structure has 2 part of it, one is the Lattice; the same Lattice can have different types of Basis actually and thus can have different types of crystal structure. So the crystal structure consists of the Basis and the Lattice.

(Refer Slide Time: 19:55)



Types of Lattice

Triclinic

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma$

$V = abc\sqrt{1 - cos2\alpha - cos2\beta - cos2\gamma + 2cos\alpha cos\beta cos\gamma}$

Monoclinic

$a \neq b \neq c$

$\alpha = \gamma = 90^0, \beta \neq 90^0$

$V = abc \sin\beta$

Orthorhombic

$a \neq b \neq c$

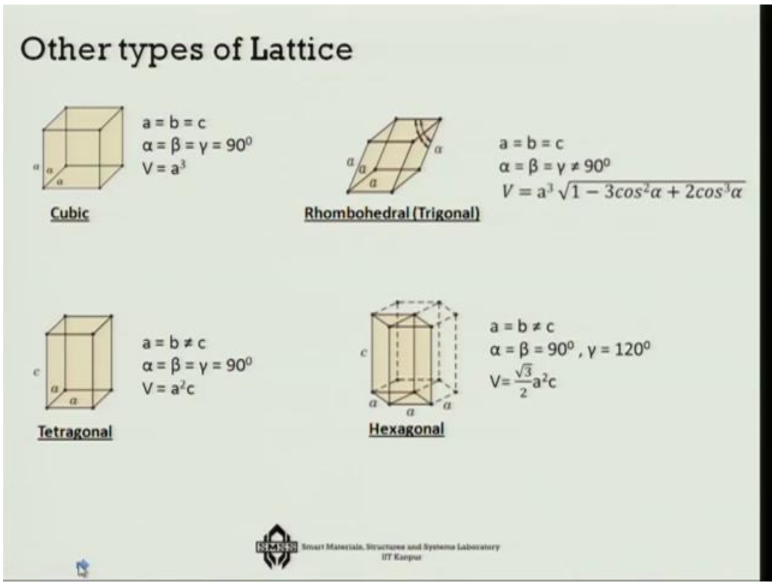
$\alpha = \beta = \gamma = 90^0$

$V = abc$

So with this background, if we go to the types of Lattice, then the 1st generic Lattice called the triclinic Lattice structure. Now, in the triclinic Lattice, these edges a, b and c, they are not equal to each other, neither the angles Alpha, Beta and Gamma. So when you have no similarity between the angles and the edges are not same okay, then you get the most generic system which is known as the triclinic system and you can find out through geometric relationship you can find out, what is the volume of a triclinic system?

From there if you bring a little more symmetry, you can get a situation where a, b, c are not equal to each other that is fine, but at least Alpha and Gamma are 90 degree okay. So Alpha and Gamma are 90 degree angles okay and Beta is not 90 degree. So then you get a structure which is known as a monoclinic structure. Now, if you get a structure where Alpha, Beta, Gamma all are 90 degree, but still a, b, c are not equal, then you get a structure which is known as Orthorhombic structure.

(Refer Slide Time: 21:22)



Other types of Lattice

$a = b = c$
$\alpha = \beta = \gamma = 90^0$
$V = a^3$

Cubic

$a = b = c$
$\alpha = \beta = \gamma \neq 90^0$
$V = a^3\sqrt{1 - 3cos^2\alpha + 2cos^3\alpha}$

Rhombohedral (Trigonal)

$a = b \neq c$
$\alpha = \beta = \gamma = 90^0$
$V = a^2c$

Tetragonal

$a = b \neq c$
$\alpha = \beta = 90^0$, $\gamma = 120^0$
$V = \frac{\sqrt{3}}{2}a^2c$

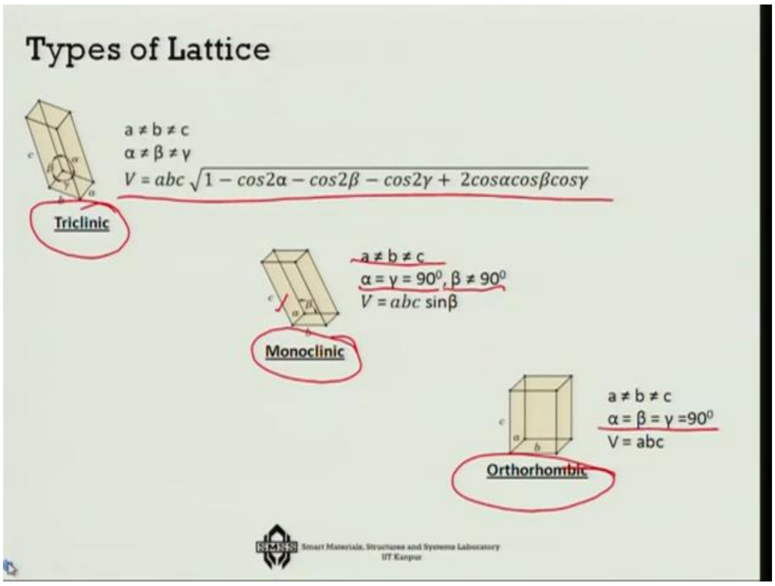
Hexagonal

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

Gradually we are introducing more and more symmetry into the parameters. So what if a, b, c are all equal and Alpha, Beta, Gamma are all 90 degree, and then you get the simplest structure which is called the cubic structure. What is a, b, c are all equal, but alpha, beta, gamma are not equal to 90 degree, then you get a Rhombohedral or a trigonal structure. What if a and b are equal, but they are not equal to c, but alpha, beta, gamma equals to 90 degree, you get a structure which is known as Tetragonal Lattice structure.

And what if a and b are equal, but they are not equal to c just like tetragonal and Alpha and Beta are only 90 degree, but gamma equals to 120 degree, then you get a structure which is known as hexagonal Lattice structure. So that means you have defined about 7 structures, okay. So that means triclinic, monoclinic, orthorhombic, cubic, Rhombohedral or trigonal, tetragonal and hexagonal structure.

(Refer Slide Time: 22:16)



Types of Lattice

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma$

$V = abc\sqrt{1 - cos2\alpha - cos2\beta - cos2\gamma + 2cos\alpha cos\beta cos\gamma}$

Triclinic

$a \neq b \neq c$

$\alpha = \gamma = 90^0, \beta \neq 90^0$

$V = abc \sin\beta$

Monoclinic

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90^0$

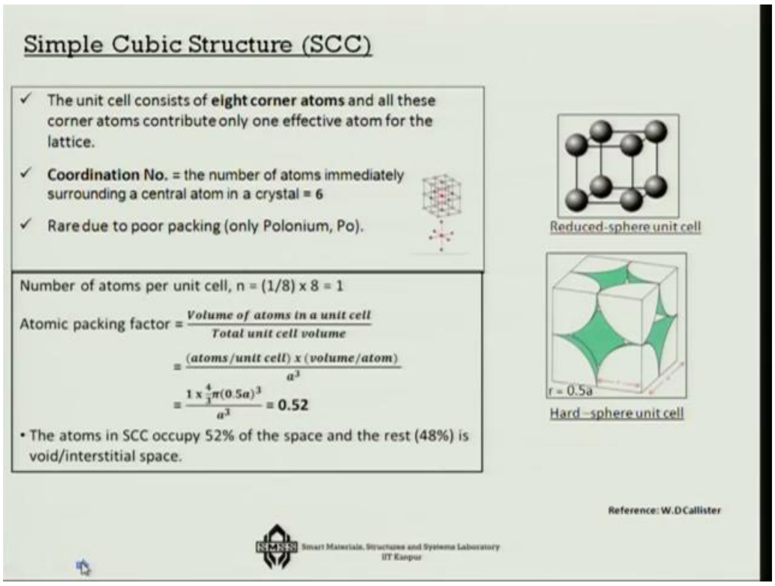
$V = abc$

Orthorhombic

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

These are the 7 basic crystal systems that is what it is called okay. The 7 basic crystal systems and if you summarize, you will once again see each one of them with cubic structure having the highest degree of symmetry and triclinic having the lowest kind of symmetry in the structure, where neither a, b, c are equal nor Alpha, beta, gamma are equal, not at all they are orthogonal, et cetera.

(Refer Slide Time: 23:08)



Simple Cubic Structure (SCC)

- ✓ The unit cell consists of **eight corner atoms** and all these corner atoms contribute only one effective atom for the lattice.
- ✓ **Coordination No.** = the number of atoms immediately surrounding a central atom in a crystal = 6
- ✓ Rare due to poor packing (only Polonium, Po).

Number of atoms per unit cell, n = (1/8) x 8 = 1

$$\text{Atomic packing factor} = \frac{\textit{Volume of atoms in a unit cell}}{\textit{Total unit cell volume}}$$

$$= \frac{(\textit{atoms/unit cell})\ x\ (\textit{volume/atom})}{a^3}$$

$$= \frac{1 \times \frac{4}{3}\pi(0.5a)^3}{a^3} = 0.52$$

- The atoms in SCC occupy 52% of the space and the rest (48%) is void/interstitial space.

Reduced-sphere unit cell

Hard-sphere unit cell

Reference: W.D Callister

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

That is what is kind of all the things, a generic map together. Now, let us look at some of the crystal structures okay. Out of these 7 crystal structures, we will take only 3 or 4 of our interest, which we generally find more in terms of the materials that we use okay. So let us 1st think of a simple cubic structure, okay.

Now, naturally in the cubic structure if you look at it very carefully, you will see that it consists of 8 corner atoms, 1, 2, 3, 4, 5, 6, 7, 8, so there are 8 corner atoms. And basically since each atom is shared by the neighboring Lattice if you look at it, there are 6 Lattices. If you consider each one of them, then each direction like this direction one, there it is getting shared, it is getting shared in this direction 2, it is getting shared in this direction 3, it is getting shared 4, 5 and 6, so like that there are 6 directions, so its coordination number okay.

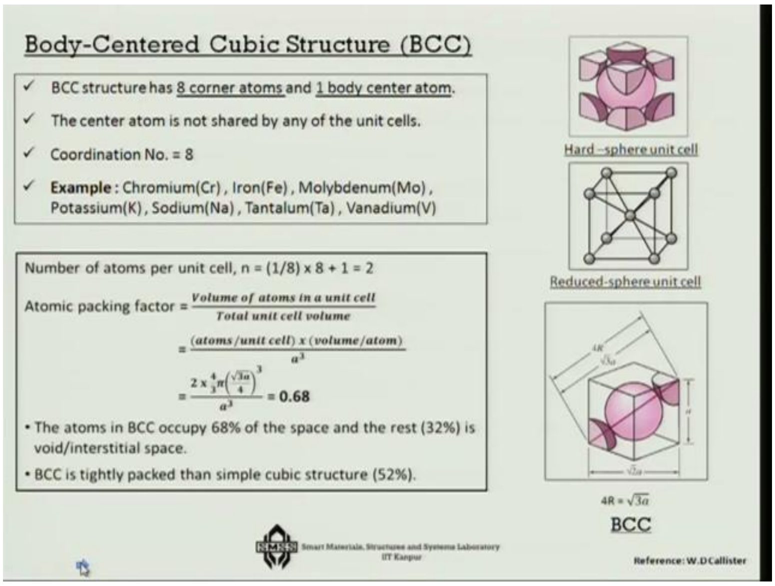
So that means, the number of atoms immediately surrounding a central atom is actually 6, so that is all is the coordination number. This type of items if you try to find out, what is the packing, that means number of atoms per unit cell, then you can do it in this manner that already that there are 8 atoms, okay and also that each one of the atom has 1/8 way of contributing to the whole thing, so the n is unity.

And the atomic packing factor, how do we calculate it, it is basically volume of atoms in a unit cell okay divided by that unit cell volume itself. Now in this case, it is a cubic okay Lattice. So that the cubic Lattice one typical geometric dimension is a, then it will be a cube, that is fine. Now, how do we find out the volume of atoms in a unit cell?

To do that, we have to find out how many atoms are there for unit cell and then the volume per atom okay. So, in this case you can find out that atom per unit cell is actually the number of atoms that 1/8 into 8, so it is effectively one. And the volume per atom, you can consider it to be a rigid spherical system without much loss of generality and you can find it out that in terms of this packing, it will be 4 by 3 pie r cube, where r is half of the a, half of the Lattice distance.

So the packing is something like 0.52 or 52% of the space. So that means in the cubic structure cubic crystal structure, 52% of the space is only occupied by the atom and the rest are actually void or interstitial space. This is a really very poor packing something like materials like polonium shows this kind of a packing system. Let us go to system which is slightly more packed.

(Refer Slide Time: 26:19)



Body-Centered Cubic Structure (BCC)

- ✓ BCC structure has 8 corner atoms and 1 body center atom.
- ✓ The center atom is not shared by any of the unit cells.
- ✓ Coordination No. = 8
- ✓ **Example** : Chromium(Cr) , Iron(Fe) , Molybdenum(Mo) , Potassium(K) , Sodium(Na) , Tantalum(Ta) , Vanadium(V)

Number of atoms per unit cell, n = (1/8) x 8 + 1 = 2

$$\text{Atomic packing factor} = \frac{\text{Volume of atoms in a unit cell}}{\text{Total unit cell volume}} = \frac{(\text{atoms/unit cell}) \times (\text{volume/atom})}{a^3} = \frac{2 \times \frac{4}{3}\pi\left(\frac{\sqrt{3}a}{4}\right)^3}{a^3} = 0.68$$

- The atoms in BCC occupy 68% of the space and the rest (32%) is void/interstitial space.
- BCC is tightly packed than simple cubic structure (52%).

$4R = \sqrt{3a}$

BCC

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

Reference: W.D Callister

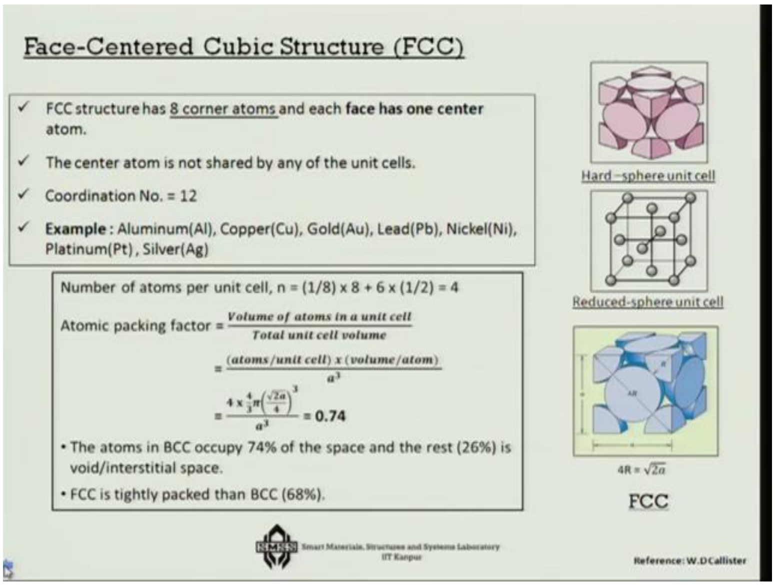
The next example is BCC Body Centered Cubic Structure. It has actually 8 atoms at the corner, 1, 2, 3, 4, 5, 6 like that it has 8 atoms if you consider the other corner 7 and the other one which you cannot see, so it atoms in the corner and 1 body Centre atom. The Centre atom is not shared many other unit cells, but all the other items are shared.

So basically if you consider the number of atoms per unit cell, then 1/8 into 8 for those atoms which are shared + the center atom, so you will get the n as 2. So then the atomic packing factor how would you count it, in this case you will see that the atoms per unit cell is 2 and once again it has the basic structure which is cubic, so it is a cube as the volume of the unit cell.

And you can find out from geometry if you look at this entire structure, you can find out that in the most compact condition the volume per atom is 4 by 3 pie times okay the root 3 a by r. That means this volume is actually the distance is root 3 a hence, this root 3 a by r 4 cube. So that if you calculate, you will see that this ratio will come out to be 0.68 that means 68% of the space is now occupied.

And 38% space will remain as a void or as an interstitial space. So compare this with a simple cubic structure which has only 52% space, so naturally this is a much more compact system. Let us look at another structure and that is Face Centered Cubic Structure FCC.

(Refer Slide Time: 28:18)



Face-Centered Cubic Structure (FCC)

- ✓ FCC structure has 8 corner atoms and each **face has one center** atom.
- ✓ The center atom is not shared by any of the unit cells.
- ✓ Coordination No. = 12
- ✓ **Example** : Aluminum(Al), Copper(Cu), Gold(Au), Lead(Pb), Nickel(Ni), Platinum(Pt) , Silver(Ag)

Number of atoms per unit cell, n = (1/8) x 8 + 6 x (1/2) = 4

$$\text{Atomic packing factor} = \frac{\textit{Volume of atoms in a unit cell}}{\textit{Total unit cell volume}}$$

$$= \frac{(\textit{atoms/unit cell}) \times (\textit{volume/atom})}{a^3}$$

$$= \frac{4 \times \frac{4}{3}\pi\left(\frac{\sqrt{2}a}{4}\right)^3}{a^3} = \mathbf{0.74}$$

- The atoms in BCC occupy 74% of the space and the rest (26%) is void/interstitial space.
- FCC is tightly packed than BCC (68%).

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

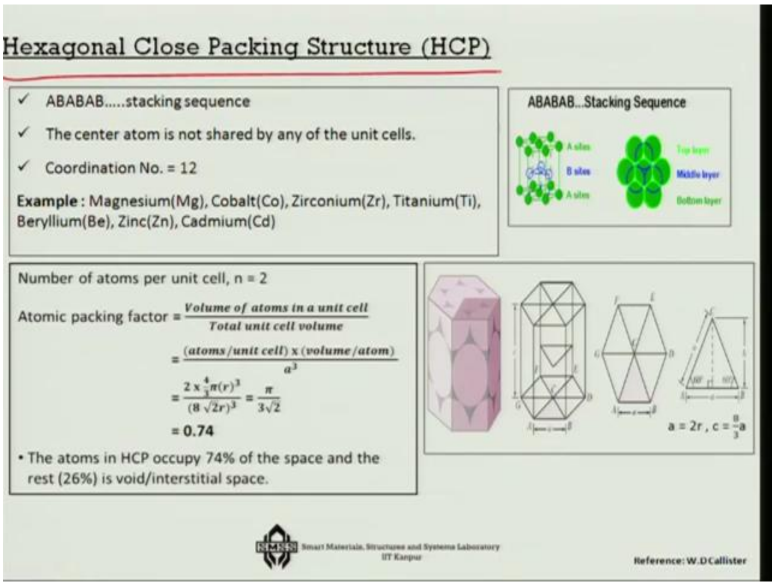
Reference: W.DCallister

In this case, you have the centre atom which is not shared okay and you have the face centered atoms also. So if you look at it that you have the corner atoms, which are giving 1 8th thing to 8 okay because you have 8 corner atoms and then you have atoms at the face centre each face centre, so that is actually 6 into half. So if you consider all of them together, you will get the number of atoms per unit cell to be 4 okay.

And then if you again calculate the whole thing, you will find out the ratio to be 0.74. That means, 74% of the space is occupied and the rest 26% is void or interstitial space. So this is definitely much more packed than even the BCC, so something like materials like Aluminium, Copper, Gold, Lead, Nickel, Platinum, Silver, they all of them show the FCC structure.

In fact, some materials can actually change their crystal structure with respect to temperature, so there is a phase transition and crystal structure change can occur in materials, best example is iron itself, we will see that. Now the other the last packing structure, which is also important, is known as the Hexagonal Close Packing Structure HCP.

(Refer Slide Time: 29:43)



Hexagonal Close Packing Structure (HCP)

- ✓ ABABAB.....stacking sequence
- ✓ The center atom is not shared by any of the unit cells.
- ✓ Coordination No. = 12

Example : Magnesium(Mg), Cobalt(Co), Zirconium(Zr), Titanium(Ti), Beryllium(Be), Zinc(Zn), Cadmium(Cd)

ABABAB...Stacking Sequence

Number of atoms per unit cell, n = 2

$$\text{Atomic packing factor} = \frac{\textit{Volume of atoms in a unit cell}}{\textit{Total unit cell volume}}$$

$$= \frac{(\textit{atoms/unit cell}) \times (\textit{volume/atom})}{a^3}$$

$$= \frac{2 \times \frac{4}{3}\pi(r)^3}{(8\sqrt{2}r)^3} = \frac{\pi}{3\sqrt{2}}$$

$$= \mathbf{0.74}$$

- The atoms in HCP occupy 74% of the space and the rest (26%) is void/interstitial space.

$a = 2r$, $c = \frac{8}{3}a$

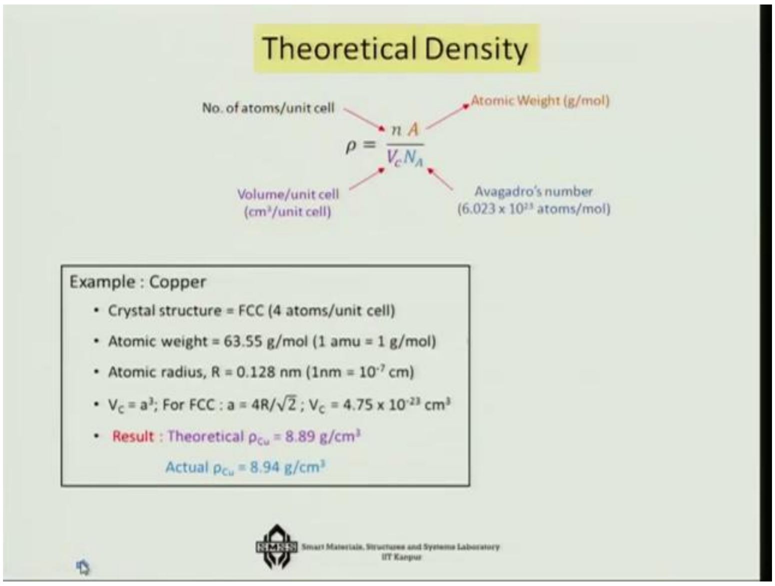
Smart Materials, Structures and Systems Laboratory
IIT Kanpur

Reference: W.D Callister

HCP has a ABABAB kind of a stacking sequence, but this stacking sequence is such that now you do not have one type of a plane, you have A type and you have to B type again A type and then again B type, that is how you are stacking each one of them. So in such a case, the number of atoms per unit cell will come out to be n equals to 2 and if you calculate the volume, you will see that this is about 0.74 that means 74% of the space is occupied and only 26% is free.

So that means this is the densest stacking sequence okay. And materials which shows this is, Magnesium, Cobalt, Zirconium, Titanium, Beryllium, Zinc, Cadmium like that. Interestingly, some of these materials are also very high in terms of density. For example, Titanium is much denser than Steel or say for Iron; so that that is possible due to the Hexagonal close packing structure.

(Refer Slide Time: 30:53)



Theoretical Density

No. of atoms/unit cell

Atomic Weight (g/mol)

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

Volume/unit cell
(cm³/unit cell)

Avagadro's number
(6.023×10^{23} atoms/mol)

Example : Copper

- Crystal structure = FCC (4 atoms/unit cell)
- Atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- Atomic radius, R = 0.128 nm (1nm = 10^{-7} cm)
- $V_C = a^3$; For FCC : $a = 4R/\sqrt{2}$; $V_C = 4.75 \times 10^{-23}$ cm³
- Result : Theoretical $\rho_{Cu} = 8.89$ g/cm³

  Actual $\rho_{Cu} = 8.94$ g/cm³

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

How to actually calculate the theoretical density that is a very interesting way, we can actually do it and one can show that for metals it matches more or less with the entire estimation of the system. So how do we do it? You need to know 2 things to do it, so density is basically mass per unit volume, so you have to calculate the mass and then you have to calculate the unit volume, so how we can do it?

You know the volume per unit cell okay for different crystal structures and that what is the packing structure for a particular material, so V c is known to us. So now how many atoms can you expect per mole that is also defined by the Avogadro's number? So we know that in terms of the number of atoms you have the number of atoms per unit cell okay.

So and also you have the atomic weight okay, which give you the mass in terms of gram per mole. So you have the atomic weight as gram per mole, okay. And you have the Avogadro's number as atoms per mole you are dividing, so this mole and mole gets cancelled and what you are getting is something like a gram per atom. So per the weight of each of the individual items you are getting.

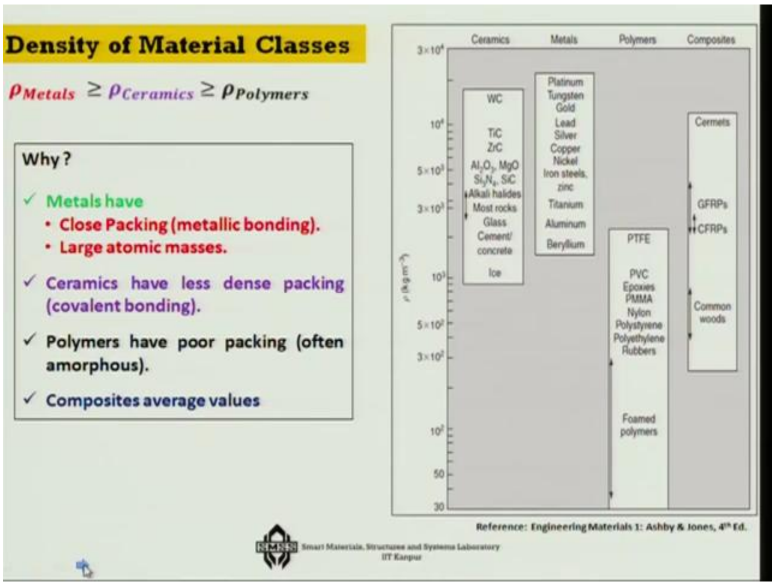
Now the number of atoms you know, so that you multiply by the weight of the each individual atom, you get the total weight of the system and the volume, so you should be able to calculate the density of the system. Let us try to use it for a simple material like copper okay. Copper structure is FCC and it has you can find out that FCC has 4 atoms per unit cell.

Now, what is atomic weight of copper? That is 63.55 grams per mole. And what is the atomic radius that is about 0.128nanometre from x-ray crystallography and such things you can find out that what the atomic radius of a system is. Now what is the volume of the system because what is a to R relationship for an FCC structure and since R is already known to you, so you should be able to find out a, so you should be able to find out what is V c.

And you mean this V c will come out to be 4.75 into10 to the power minus 23 cm, a very small work, but nevertheless we are talking in the in the crystal structure level. So we know the volume okay and you also know the weight, so if you calculate you will see the theoretical density will come out to be 8.89 gram per cm cube. In fact, density of the pure copper is about 8.94, so that means theoretical density calculation is quite close to what it should be in practice.

So that is how we can that what has contributed to this density of atom, the crystal structure has contributed to the density of atom other than all other things like atomic weight, atomic radius, et cetera. So thus if the crystal structure, you can actually predict that what is the kind of density that you can expect from a particular structure.

(Refer Slide Time: 34:28)



Density of Material Classes

$\rho_{Metals} \geq \rho_{Ceramics} \geq \rho_{Polymers}$

Why ?

- ✓ Metals have
  - Close Packing (metallic bonding).
  - Large atomic masses.
- ✓ Ceramics have less dense packing (covalent bonding).
- ✓ Polymers have poor packing (often amorphous).
- ✓ Composites average values

Reference: Engineering Materials 1: Ashby & Jones, 4th Ed.

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

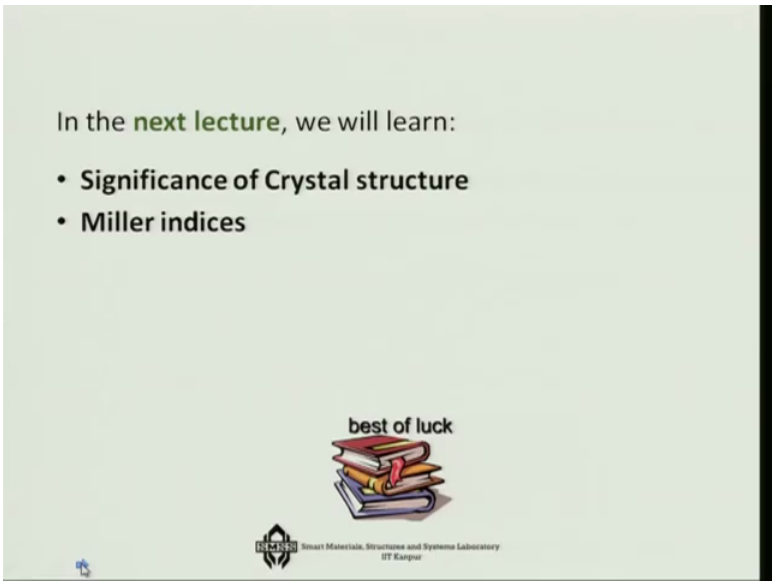
Now the density of various material classes if you have look at it, you will see that in the high-density region, we will mostly see most of the metals okay, like Tungsten, Gold, Lead, they are having very density, then Titanium, Aluminium, Beryllium, et cetera. And a similar type of density, I will talk about it in terms of ceramics at a later talk, also you will see that they are also comparable density wise.

But if you look at the polymers, they really have very low density, because you see they have the amorphous structure. Since they have amorphous structure, so they have very poor packing and since they have very poor packing even though they consist of some of the very similar atoms, but they have a very low density.

So that is why we say that metals have higher density because it has close packing and also individual atomic masses are generally more. Ceramics have less dense packing in comparison to the metals okay and polymers have the poorest packing that is why they are amorphous and hence you see that their density is much lower.

And composites, since they are mixed of these things, so they are somewhere in middle because they may have some ceramics and some polymers that is why they are somewhere kind of an average property you will be in the composites. So that is how typically from the structure, the crystal structure you can actually predict that what is going to be the density of the system.

(Refer Slide Time: 36:15)



In the **next lecture**, we will learn:

- **Significance of Crystal structure**
- **Miller indices**

best of luck

Smart Materials, Structures and Systems Laboratory
IIT Kanpur

This is where we will close today and in the next lecture we will learn the significance of crystal structure further and something very important to describe such a system, which is known as the Miller indices, thank you.