

Basics of Mechanical Engineering-2

Prof. J. Ramkumar

Prof. Amandeep Singh Oberoi

Department of Mechanical Engineering

Indian Institute of Technology, Kanpur

Week 02

Lecture 05

Crystal Structures

Students, welcome to the next lecture on Crystal Structure. In the first week, we saw different types of materials: ferrous, non-ferrous. We also saw alloys, composites, and polymer materials. Now, where does this difference come from? The big difference comes from the crystal structure.

So now, in the first lecture of this week, we will try to understand the crystal structure. We will divide the lecture into two parts. We will have the theory covered by me, and the problem-solving will be done by Dr. Amandeep. So, each lecture's theory will be backed by problem-solving. So that you understand and appreciate the course.

Contents

- Crystal Structure
- Crystalline Solid
 - Single Crystal Solid
 - Poly Crystal Solid
- Non-crystalline Solids
- Space Lattice
- Unit Cell
- Atomic Packaging Factor
- Co-ordination Number
 - Simple Cubic
 - Face Centered Cubic
 - Body Centered Cubic
- Recapitulate



In terms of content, we will first start with Crystal Structure. Then, Crystalline Solids: single-crystal solid, polycrystal solid. The majority of the materials available will be polycrystal solids. Then, we also have Non-Crystalline Solids. So, where does this crystal come into play in a big way? It's in the Space Lattice.

We will understand what a Unit Cell is, which is nothing but a building block for a complete material. Then, how are these building blocks packed? So, we will try to see the Atomic Packing Factor. Then, the Coordination Number. We will try to cover three simple factors.

Cubic structures: simple cubic, face-centered, and body-centered. However, there are seven basic ones, so we will try to cover three and maybe one or two more additional ones during the problem-solving class. And finally, we will try to have a recap.

Crystal Structure

Introduction

- Crystallography is the experimental science of determining the arrangement of atoms in crystalline solids.
- Groups of atoms/molecules specifically arranged called crystals.



<https://www.gemsociety.org/article/crystallography-introduction-mineral-crystal-systems/>

3

Crystal Structure. Crystallography is an experimental science of determining the arrangement of atoms in crystalline solids.

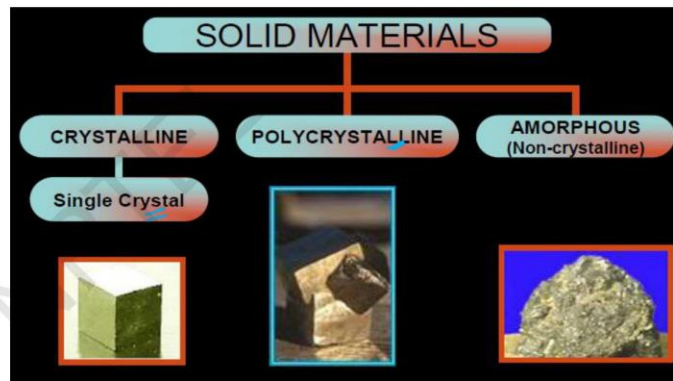
People talk about crystallography in a big way. The big difference between artificial diamond and original diamond is understanding the crystallography. Groups of atoms or molecules specifically arranged are called a Crystal. So, the study of it is Crystallography. So, crystallographers study crystal structure.

This is an area that is coming up in a big way. Because we are trying to look at exotic materials that have combinational properties, or we have hit the limits of various materials. So now we are trying to dope with some atoms so that the crystal structure can be modified a little bit.

Crystal Structure



- All solid materials are made of atoms/molecules arranged in a specific order in some materials, called crystalline solids. Otherwise, non-crystalline or amorphous solids.



So when we take any solid material, it is classified as crystalline, polycrystalline, or amorphous. Crystalline means it is a single crystal.

Today, we talk about single-crystal titanium material for turbine blade applications because of their excellent mechanical properties. Polycrystalline materials are various crystals put together to form a single object. Amorphous materials are non-crystalline materials. Many of the polymers are amorphous in nature. Many of the glass materials are amorphous in nature.

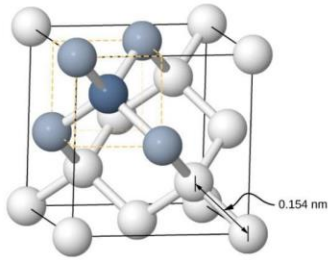
All solid materials are made of atoms or molecules arranged in a specific order in some materials called crystalline solids. If the arrangement is not there, it is otherwise called non-crystalline or amorphous material. So basically, the building block is atoms, atoms to unit cell. Atoms are the smallest known materials for us. So again, you can see electrons, protons, and neutrons are there.

But to a large extent, from the metallurgy point of view, we always try to talk about only atoms. So these are atoms. These atoms are arranged in some fashion. So if they are arranged in an orderly fashion, it is called a crystalline solid.

Crystal Structure



Principal forms of solid structures



Crystalline solids



Non-crystalline (amorphous) solids

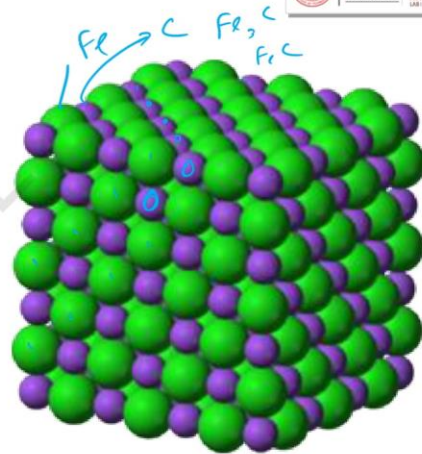


<https://www.alamy.com/stock-photo/non-crystalline.html?sortBy=relevant>
<https://pressbooks.online.ucf.edu/osuniversityphysics3/chapter/bonding-in-crystalline-solids/>

The principal form of solid structures is crystalline. You see these are all the atoms. These atoms are bonded together, and these atoms can be arranged in a unit cell. So this is called a unit cell. So this is a crystalline solid, and here you see non-crystalline or amorphous material. How does it look?

Crystalline Solids

- Crystalline bodies are characterized by an ordered arrangement of their ions, atoms or molecules.
- Its a substance in which the atoms or molecules are arranged in a definite, repeating pattern in three dimension.
- Metals normally form crystalline solids, but some ceramic materials are crystalline.

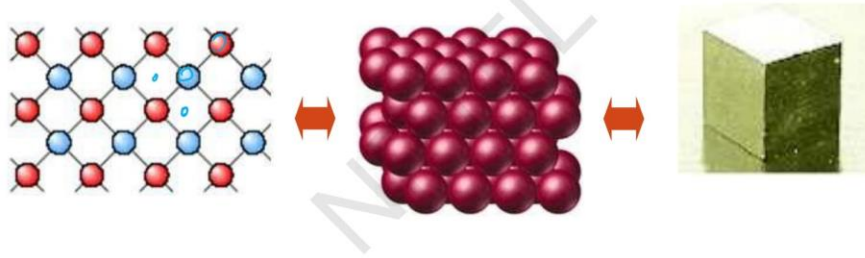


The crystal structure, how does it look? So crystalline solids are characterized by the ordered arrangement of their ions, atoms, and molecules. This green one is orderly arranged, and you can see these violet atoms, which are nothing but diffused atoms between the basic atoms. This can be iron; all green can be iron, and all violet can be carbon. So it forms Fe_3C or FeC .

So it is a substance in which the atoms or molecules are arranged in a definite repeating pattern in three dimensions. Metals normally form crystalline solids, but some ceramics are also crystalline. So you should also understand this. Ceramic materials can also be crystalline.

Crystalline Solids

- The spatial arrangement of their ions, atoms or molecules, and on the composition, size and shape of crystals.



The spatial arrangement of their ions, atoms, or molecules and the composition, size, and shape of the crystal you can try to form.

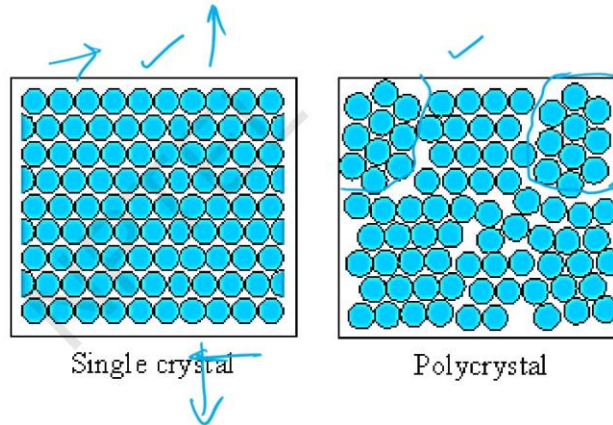
So these are 2D forms, these are 3D forms, and this is the total solid which you see in reality. These two are seen in the microscopic views. So the spatial arrangement of their ions, atoms, these are all atoms or molecules, and on the composition, so this is the composition, red one and blue one composition, size, the shape and size of this. So if the atom has to be joined here, it has to be equisized or have a difference of maybe 10% variation. Generally, what happens is, it always sits in between. So composition, size, and shape of the crystal are very important.

Crystalline Solids: Type



Crystalline solids are classified into two types

- Single crystal (Periodic across the whole volume)
- Poly crystal (Periodic across each grain)



So this is a single crystal, and this is a polycrystal. Single crystals have a periodic arrangement across the whole volume. Polycrystalline materials have a periodic arrangement across a grain. So this is a grain.

So if you see here, this is a grain. So inside a grain, they have a crystal structure or a uniform arrangement. But between grains, there can be different arrangements. When you talk about a single crystal, it is uniformly arranged across the whole volume. So what is the advantage?

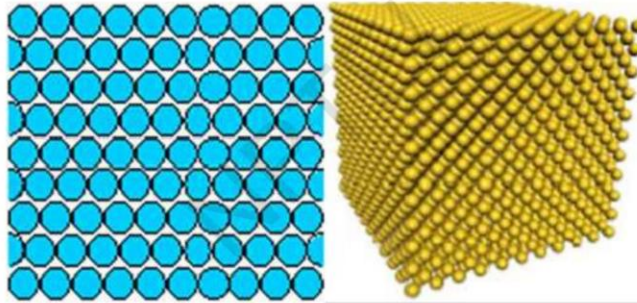
When I try to pull or push, tensile, compression, shear, I get wonderful mechanical performance. I can now dictate the material such that it meets the application. And how do you get this? You play with heat treatment, which we will discuss in the upcoming lectures. Right? So now, I am sure you should be able to clearly understand crystalline and non-crystalline.

In non-crystalline, polycrystalline and amorphous. So these are polycrystalline materials.

Crystalline Solids: Single Crystal → Si



- Even at infinite length scales, each atom is related to every other equivalent atom in the structure by translational symmetry.

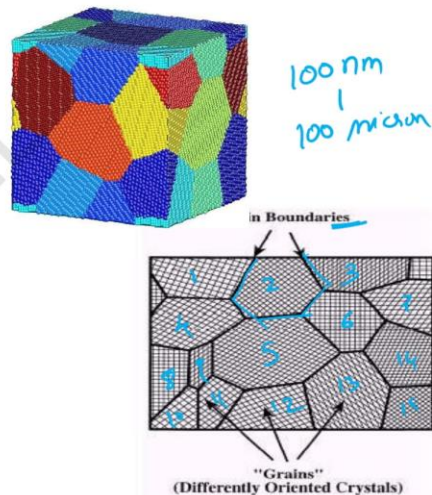


So when we talk about a single crystal, a single crystal is a silicon material. We talk about a single crystal. Even at an infinite length scale, each atom is related to every other equivalent atom in the crystal by translational symmetry. So this is seen in single crystals. In silicon, you can have single crystals.

Crystalline Solids: Polycrystal



- Its a material made up of an aggregate of many small single crystals.(also called crystallites or grains)
- The grains are usually 100 nm - 100 microns in diameter.
- Polycrystals with grains that are < 10 nm in diameter are called nano-crystalline.



When we talk about polycrystalline, It is a material made up of an aggregate of many small-sized crystals. So you can see here, this is a grain, and around the grain, it is covered by a boundary called the grain boundary.

So the grain boundary has a lot of energy. So when you try to etch it, it forms a depth. That's why, when you see it in a microscopic image, you see a black color at the grain boundary. So each of these grains will have different arrangements. All these things put together will be there in one material.

So the grains are usually 100 nanometers to 100 microns. So again, how do you play with the grain size? When you do heat treatment, we play with the grain size. Polycrystalline materials with grain sizes that are less than 10 nanometers in diameter are called nanocrystalline. So the size we are talking about is 100 nanometers to 100 microns. This is normal.

When we go towards 10 nanometers, it is called nano-crystalline material. Nano-crystalline material has different properties. For example, gold behaves differently at 100 nanometers compared to 10 nanometers in terms of optical properties. It is different. Mechanical properties are different.

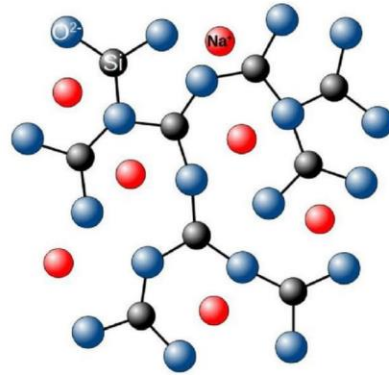
Thermal properties are different. That is why we say nano-crystalline. Polycrystalline is further divided into nano-crystalline. Nano-crystalline materials are the talk of the town now. Now, they are trying to make inserts, cutting tool inserts of nano-grains.

They are trying to make nano-crystal materials on top of alloys such that they have good heat extraction properties. Nano-crystalline is gaining momentum today.

Non-crystalline Solids



- Non-crystalline solids are also known as **amorphous solids**.
- In an amorphous solid atoms do not possess well defined arrangement (atoms have no periodic packing).
- Amorphous structures form in complex structures, polymers, and rapidly cooled materials.
- In non-crystalline solids, particles have a little freedom to move since they are not arranged rigidly as in other solids.



https://www.researchgate.net/figure/Glass-structure-at-the-atomic-level-Oxygen-and-silicon-atoms-form-a-network-which-is_fig1_283303190 11

Non-Crystalline Solids. Non-Crystalline Solids are also called amorphous solids. In an amorphous solid, atoms do not possess a well-defined arrangement.

If you look at it, it does not possess a regular arrangement. So what is the difficulty? If it does not possess a regular arrangement, then if you want to tweak the material to meet the engineering requirements, it is difficult. But in reality, these are the things which can easily be formed. So amorphous solids have their own advantages.

Amorphous structures form in complex structures, polymers, and rapidly cooled materials. So it is used in glass. So amorphous structures form in complex structures in polymers like thermoplastics, thermosets, and elastomers. You also have glass with this property, and they are rapidly cooled. In non-crystalline solids, the particles have little freedom to move, since they are not arranged rigidly as in other solids.

So amorphous solids, polymers also come. So thermoset polymers are also there. So there is not much freedom for movement. So if you look at the volume to unit weight, With respect to time, you can see how the response is.

So, volume per unit weight with respect to time. Why is this important? Because later in your manufacturing process, we will see casting and injection molding, where the starting material will be a liquid. So, if it is a liquid, how does it respond for a crystalline

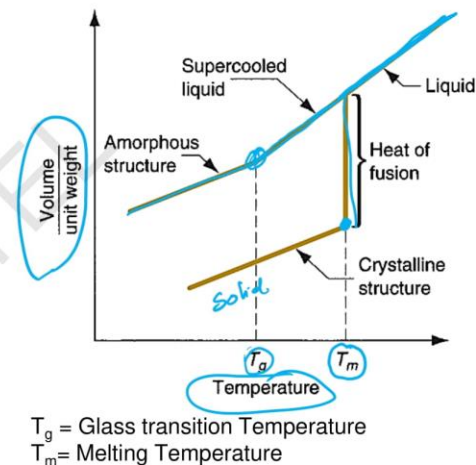
structure and for a non-crystalline or amorphous structure? So, if you see that for a crystalline structure, it has a sharp melting point.

So, as the temperature increases, at one particular point, there is a melting point. And then you can see that there is a heat of fusion, and then it becomes a liquid. So, this is solid; there is a transition, and then it forms a liquid. Whereas, when you try to take an amorphous material or a non-crystalline material, it has an amorphous structure. So, there is not much change in the temperature profile.

So, that means to say, there is no sharp transition. So, you see here, an amorphous structure. Then, as and when you keep increasing the temperature, it takes you to a supercooled liquid, and then it becomes a liquid. So here, where exactly the change in slope happens, this point is called the glass transition temperature. So, generally, for a polymer material, we always call it the glass transition temperature point, wherein there is a change in weight to unit volume as compared to that of a crystalline material. Keep this in mind. Because this information will be very useful when we see the casting process or when we see the injection molding process during the course.

Non-crystalline Solids

- An amorphous material exhibits quite different behavior than that of a pure metal when it changes from solid to liquid.
- The Characteristic change in volume for a pure metal (a crystalline structure), compared to the same volumetric changes in glass (a non-crystalline structure).



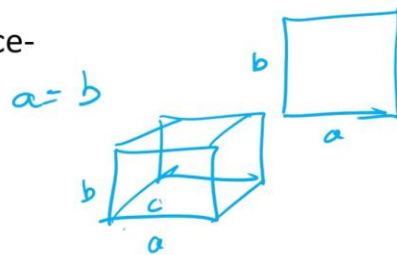
An amorphous material exhibits quite different behavior from the pure metal when it changes from solid to liquid. So there is also an expansion. Please understand. So why is this expansion very important? Later, when you try to convert this liquid into solid, there will be a contraction of the material.

That concept we will see in casting. The characteristics change in the volume of a pure metal compared to the same volumetric change of the glass, you can see a difference. So now, friends, you will try to understand why the melting point is important. Why is the glass transition temperature point important? And why are we so much worried about crystalline and non-crystalline materials?

Space Lattice



- A three-dimensional translational periodic arrangement of points in space is called a lattice.
- An infinite array of points in three dimensional in which every point has an identical environment to all others is called a space lattice.
- There are two types of space lattice-
 - Square space lattice($a=b$)
 - Cubic space lattice($a=b=c$)



13

So now, let us understand the Space Lattice. Because until now, what we were trying to discuss, we were trying to see atoms. These atoms are getting arranged. This is what we saw. But now let us understand in three-dimensional space, what is it?

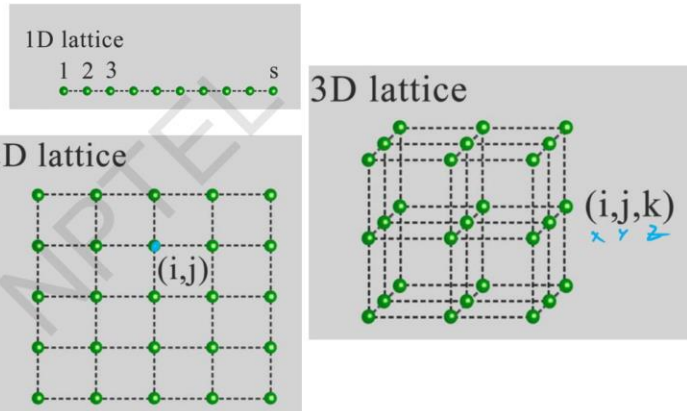
So we are now getting into space lattice. A three-dimensional translational periodic arrangement of points in space is called a lattice. An infinite array of points in three-dimensional space in which every point has an identical environment to all others is called a spatial lattice. So now, we are trying to look into how the atoms are arranged in the given space. So a periodic arrangement of points, where every point has an identical environment to all others, is called a spatial lattice.

There are two types of spatial lattice. One is called a square spatial lattice. The other one is called a cubic spatial lattice. A equals B . We will see that and then A equals B equals C . So what are we trying to say?

This is A and B . When we try to talk about a cube, A , B , and C .

Space Lattice

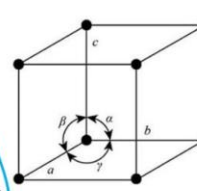
- Space lattice can also be classified on the basis of dimensions-
 - 1-D space lattice
 - 2-D space lattice
 - 3-D space lattice



Spatial lattice can also be classified on the basis of dimensions. This is 1D. This is what we were discussing: 2D and this is 3D. When we define a point i, j . So this is 1D, only i . This is i, j and this is i, j, k . So you have x, y , and z . The spatial lattice can also be classified on the basis of dimensions. So what we saw here, there are two types of spatial lattices: square and cube. So here you can see one-dimensional space lattice, two-dimensional space lattice, and three-dimensional space lattices.

Metallic Crystal Structures

- Every material is a building material block to some unit called Bravais lattice. There are 7 different types of Bravais lattices.

System	Axial Length	Axial Angle	
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$	
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ, \beta \neq 90^\circ$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	

In metallic crystal structure, there are seven different types of Bravais lattices. There are many, but these are the fundamental seven. Every material is a building block of some units called Bravais lattices.

So there are seven different types of Bravais lattices. So these seven are important. It is good that you understand and can also memorize them. Cubic, where A equals B equals C . A equals B equals C , in which the angles α , β , and γ are all at 90 degrees. When we try to draw a tetrahedron.

Tetrahedron, you are compressing and then trying to move it. So where A and B will be equal, which is not equal to C , in which the angles can be α , β , and γ , all at 90 degrees. The orthorhombic system, where A is not equal to B is not equal to C , where α , β , and γ are all 90 degrees. If you see here, they all have an angle of 90 degrees. And, if you see here, interestingly, we are trying to say length A equals B equals C , AB which is not equal to C , A not equal to B not equal to C . And now, what are the other variations? I will try to now change this angle.

When we go into rhombohedral, you will see that α equals β equals γ , which is not equal to 90. That's from the hexagon, wherein you will see α and β will be 90, and γ will be 120. So now, what are we trying to do? We are only trying to say the change in the angle. So it should be 90 or 120.

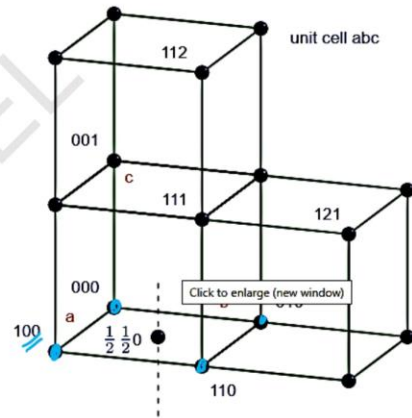
So then, when we try to see monoclinic, you see α equals γ equals 90, which is the same as the previous, whereas β is not equal to 90. So the changes, this one is not equal to 90, but these two fellows are 90. And the last one you see, triclinic, where α , β , γ , none of them are 90. Let us go to here. A equals B equals C . It is a repeat.

A equals B not equal to C . A not equal to B not equal to C . This is just a repeat. This one and this one are repeats. And then finally, it will be A not equal to B not equal to C . And here, the important points are the angles which are getting changed. So axial length and axial angle play an important role in deciding the different types of Bravais lattice. Now, why are these things important?

Cubic, tetrahedron, orthorhombic, rhombohedral, all these things have a direct influence on the physical property, mechanical property, and their service condition exposure. It is very important. That is why we are trying to understand this in more detail.

Unit Cell

- Unit cell is the basic structural unit or building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within.
- The distance from one atom to another atom measured along one of the axis is called the space constant.



https://nte.mines-albi.fr/SciMat/en/co/SM_uc1-4-2.html

16

Unit Cell. Unit Cell is the basic crystal unit or building block of a crystal structure and defines the crystal structure by virtue of its geometry and the atoms positioned within.

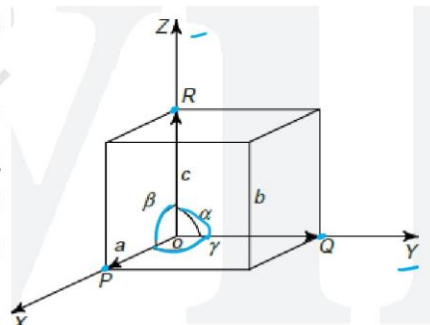
So these are all the atoms positioned within. So when we try to define this point, we try to say it is 1, 0, 0 or 0, 0, 0. These are all planes. The distance from one atom to another atom measured along one of the axes is called a space constant. So this is how a unit cell is there, and these are the planes.

Unit Cell

The unit cell is formed by primitives or intercepts a , b and c along X , Y and Z axes respectively.

A unit cell can be completely described by the three vectors, \underline{a} , \underline{b} , and \underline{c} (OP , OQ and OR) when the length of the vectors and the angles between them (α, β, γ) are specified.

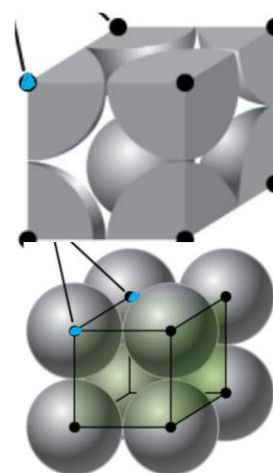
The three angles α , β and γ are called interfacial angles.



The unit cell is formed by primitives or intercepts A, B, C along the X, Y, and Z axes respectively. The unit cell can be completely described by the three vectors, A, B, and C, when the length of the vectors and the angles between them, α , β , and γ , are specified. The three angles, α , β , and γ , are called interfacial angles. So where are they? α , β , and γ , they are called the interfacial angles. And this is A, B, and C, these are the distances A in the X plane, Y plane, and Z plane respectively. At the point where they meet is P, Q, R on the XYZ coordinates.

Primitive Unit Cell

- The unit cell that contains one lattice point only at the corners is known as called primitive unit cell.
- In some cases the unit cell may coincide with the primitive cell, but in general the former differs from the latter in that it is not restricted to being the equivalent of one lattice point.
- The units cells, which contain more than one lattice point are called non-primitive cells.



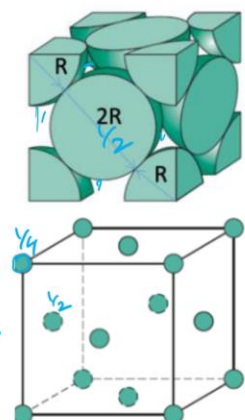
So the primitive unit cell, the unit cell that contains one lattice point only at the corner, is called the primitive unit cell. In some cases, the unit cell may coincide with the primitive cell, but in general, the former differs from the latter in that it is not restricted to being the equivalent of one lattice point. So, these two definitions' clarity is important. So, you can see here and look at this diagram, right?

The unit cell which contains more than one lattice point is called a non-primitive cell. So, primitive cell and non-primitive cells. Now, comes the question of how these atoms are getting packed inside a unit cell. What is a unit cell? It is a building block.

Atomic Packing Factor

- Atomic packing factor (APF) is defined as the percentage volume of units covered by the atoms.
- This is defined as the ratio of total volume of atoms in a unit cell to the total volume of the unit cell.
- This is also called relative density of packing (RD)

$$APF = \frac{\text{No. of atoms} \times \text{volume of one atom}}{\text{volume of unit cell}} = \frac{v}{V}$$



<https://www.transutors.com/questions/find-the-relation-between-r-and-a-b-how-many-atoms-are-in-a-face-centered-cubic-fcc-8535674.htm>

So now, let us try to understand the Atomic Packing Factor, the number of atoms which are packed inside a unit cell. So that is called the Atomic Packing Factor (APF), which is defined as the percentage volume of units covered by the atoms because there is also free space. This is defined as the ratio of the total volume of the atoms in a unit cell to the total volume of the unit cell. So we are trying to find out the volume fraction of the atoms present. You have to now clearly map your understanding with primitive unit cell and non-primitive unit cell such that you can try to understand.

This is defined as a ratio. What is defined? APF is defined as the ratio of the total volume of atoms in a unit cell to the total volume of the unit cell. So this is called the relative density of packing. So

$$APF = \frac{\text{No. of atoms} \times \text{volume of one atom}}{\text{volume of unit cell}} = \frac{v}{V}$$

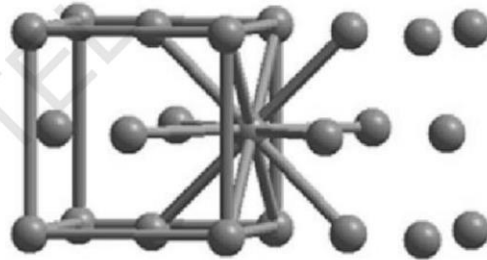
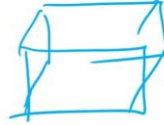
So what is the volume of an atom? So this is the volume of the atom. So you have to try to calculate the volume of a sphere. Now, the question is whether this atom sitting in the corner is sharing with four other atoms or is it sharing with another unit cell only, or how is it? The face where the atom is sitting, is it sharing another face atom, so another face plane, so that the atom can become half?

Here, it can become a quarter. Here, it is half. And suppose, if something is sitting inside, it is a full atom. So the number of atoms, these are the number of atoms, and then the volume of one atom, we know the volume of one atom, that divided by the unit cell gives

you this APF. There can be problems in the examination to calculate the APF of a unit cell which is given.

Co-ordination No.

- The number of equidistant nearest neighbouring atoms that an atom has in the given structure is known as co-ordination number.
- Co-ordination number For SC (simple cubic), BCC, FCC crystal system are 6, 8 and 12 respectively.
- Co-ordination number cannot be more than 12.



<https://homework.study.com/explanation/how-do-you-find-the-coordination-number-of-a-unit-cell.html>

20

Coordinate Numbers. This is the next important concept. The number of equidistant nearest neighboring atoms that an atom has in the given structure is known as the coordination number. So the coordination numbers for a simple cubic are BCC, we will see that.

FCC is 6, 8, and 12. The coordination numbers cannot be more than 12. So I would request you to think why this restriction is coming. So you can draw a cube. Right. And please go by the definition: the number of equidistant nearest neighboring atoms that an atom has in the given structure is called the coordination number.

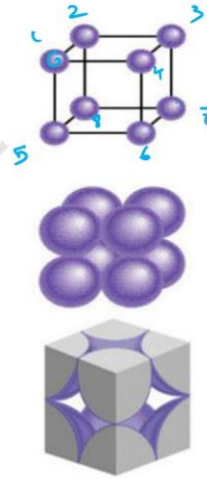
So now, you will try to figure out how this limitation is coming. This can be an exercise for you.

Simple Cubic

- There is one atom at each corner and this atom is shared by 8 unit cells. So number of atoms per unit cell.

$$n = (1/8) \times 8 = 1$$

- The coordination number of simple cubic is 6.
- Size of unit cell (lattice constant) = a



Now, let us first start looking into Simple Cubic. Simple cubic, there is one atom at each corner. 1, 2, 3, 4, 5, 6, 7, 8. There is one atom at each corner, and this atom is shared by 8 unit cells. So the coordination number will be $1/8 \times 8 = 1$.

The coordination number for a simple cubic is 6. The size of a unit cell atom is always constant as a .

Simple Cubic

$$\begin{aligned} \text{APF} &= \frac{\text{Volume of the atoms in unit cell}}{\text{Volume of the unit cell}} \\ &= \frac{\text{No. of effective atoms} \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3} \\ &= \frac{1 \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3} = \frac{\frac{4}{3} \cdot \pi \cdot r^3}{(2r)^3} = \frac{\pi}{6} \\ &= 0.52 = 52\% \text{ is filled volume} \end{aligned}$$

So,

$$\begin{aligned}
 \text{APF} &= \frac{\text{Volume of the atoms in unit cell}}{\text{Volume of the unit cell}} \\
 &= \frac{\text{No. of effective atoms} \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3} \\
 &= \frac{1 \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3} = \frac{\frac{4}{3} \cdot \pi \cdot r^3}{(2r)^3} = \frac{\pi}{6} \\
 &= 0.52 = 52\% \text{ is filled volume}
 \end{aligned}$$

Now, let us take BCC. So if you see a simple cubic, the atoms are located at the corners.

When we try to do BCC, you will see the atoms are located at the corners, and in the body center, you will have one more atom.

Body Centered Cube

- Along with one atom at each corner there is atom at the centre of each unit cell which is in physical contact with all the corner atoms.
 $n = \{(1/8) \times 8\} + 1 = 2$
- The coordination number of simple cubic is 8.
- Size of unit cell (lattice constant) = a



So now, it will be along with one atom at each corner, and there is one atom at the center. So those cells are called BCC (Body Centered Cubic). So here, apart from this simple 1 by 8 into 8, we have one more additional component. So the coordination number of a body-centered cube is 8.

Body Centered Cube

$$\text{APF} = \frac{\text{Volume of the atoms in unit cell}}{\text{Volume of the unit cell}}$$

$$= \frac{\text{No. of effective atoms} \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3}$$

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

$$= 0.68 = 68\% \text{ Filled Volume}$$

So now,

$$\text{APF} = \frac{\text{Volume of the atoms in unit cell}}{\text{Volume of the unit cell}}$$

$$= \frac{\text{No. of effective atoms} \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3}$$

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

$$= 0.68 = 68\% \text{ Filled Volume}$$

Now, you see depending upon the atom's location and you define the body-centered or whether it is simple cubic, you see the atomic packing factor changes.

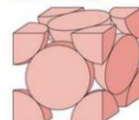
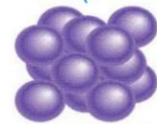
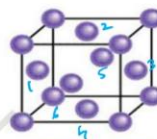
Face Centered Cube

- Along with one atom at each corner there is an atom on each face.

$$n = \left\{ \left(\frac{1}{8} \right) \times 8 \right\} + \left\{ \left(\frac{1}{2} \right) \times 6 \right\}$$

$$= 4$$

- The coordination number of simple cubic is 12.
- Size of unit cell (lattice constant) = a



Now, when we do for Face Centered. What is Face Centered? In Face Centered, you will have the basic cubic, and at every face, you will have one atom. So 1, 2, 3, 4, you will have 5 and 6.

So when you try to draw a cube, so there are 6 faces 1, 2, 3, 4, 5, and 6. So in Face Centered, at every face, you will have an atom, okay. Along with one atom at each corner, there is an atom at each face. So the coordination number of simple cubic is 12. So the constant is A.

Face Centered Cube



$$\begin{aligned}
 \text{APF} &= \frac{\text{Volume of the atoms in unit cell}}{\text{Volume of the unit cell}} \\
 &= \frac{\text{No. of effective atoms} \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3} \\
 &= \frac{4 \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3} = \frac{2 \times \frac{4}{3} \cdot \pi \cdot r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = \frac{\pi}{3\sqrt{2}} \\
 &= 0.74 = 74\% \text{ filled volume}
 \end{aligned}$$



26

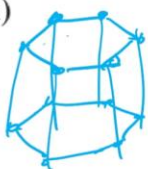
You can see there what is the atomic packing factor.

$$\begin{aligned}
 \text{APF} &= \frac{\text{Volume of the atoms in unit cell}}{\text{Volume of the unit cell}} \\
 &= \frac{\text{No. of effective atoms} \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3} \\
 &= \frac{4 \times \frac{4}{3} \cdot \pi \cdot r^3}{a^3} = \frac{2 \times \frac{4}{3} \cdot \pi \cdot r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = \frac{\pi}{3\sqrt{2}} \\
 &= 0.74 = 74\% \text{ filled volume}
 \end{aligned}$$

So with this, you can try to give some assessment about the material.

Examples

Some of the examples for the metals are given as:

Body-Centered Cubic (BCC)	Face-Centered Cubic (FCC)	Hexagonal Close-Packed (HCP)
Chromium (Cr) ✓ Iron (Fe) ✓ Molybdenum (Mo) ✓ Tantalum (Ta) ✓ Tungsten (W) ✓ 68%	Aluminum (Al) Copper (Cu) Gold (Au) Lead (Pb) Silver (Ag) Nickel (Ni) 72%	Magnesium (Mg) Titanium (Ti) Zinc (Zn) 

So now, let us see what all the metals are which fall under various cubic cells. One, BCC you will have chromium, iron, molybdenum, tantalum, and tungsten. So, 68% filling factor. You look at FCC. FCC, you will have 72% aluminium, copper, gold, lead, silver, and nickel.

So, all these are ductile materials. And these ductile materials, when you have atoms in each of these phases, then what happens is there is an easy sliding possibility. So, because of this, you will have more ductility in FCC materials. And in the tutorial, we will try to see HCP material. HCP is, you will have a hexagon on the top and then a hexagon on the bottom. You will have a hexagon on the top and then you will have a hexagon on the bottom.

Now, you will try to see each of these. Here, you will have atoms, and we will try to see how they are getting packed. So, titanium, zinc, and magnesium fall under the category of HCP. If you look more in detail, you will understand there is something called a slip plane. Then, what are the different possible slip planes?

All these details are there. But that will take us beyond the course objective. So we will stop here. All I have to tell you is, there is an atom. These atoms are arranged, and when they are arranged, it is crystalline.

If they are not arranged, it is polycrystalline. So polycrystalline means, within a crystal, there are several grains. Each of the grains can have a different arrangement. Now, let us try to take an atom. Now, how are these atoms placed inside?

So you will try to understand a unit cell. From the unit cell, we studied the atomic packing factor. From there, we also try to look into the coordination numbers. So because we are more focused on manufacturing, with this understanding, we will try to move further down.

To Recapitulate



- What are atomic structures?
- Crystalline and non-crystalline Solids
- Atomic Packaging Factor
- Co-ordination no.
- Type of structures.
- SC, FCC, BCC, etc

$CN \Rightarrow 12$



28

In this lecture, what did we recap? We recap what the atomic structures are. Crystalline, non-crystalline, atomic packing factor, coordination numbers, different types of structures, simple cubic, FCC, BCC (Body Centered). So, it is FCC and BCC, etc., that we saw. I have given you one assignment. I have asked you, why can't the coordination number be more than 12?

That's the assignment I have given. Please check and get back with the results.

References



1. Narula, G.K., Narula, K.S. and Gupta, V.K., 1989. Materials science. Tata McGraw-Hill Education.
2. Kakani, S.L., 2004. Material science. New Age International (P) Ltd., Publishers
3. Callister Jr, W.D. and Rethwisch, D.G., 2020. Materials science and engineering: an introduction. John Wiley & sons.
4. Schmid, S.R. and Kalpakjian, S., 2006. Manufacturing engineering and technology. Pearson Prentice Hall.
5. Groover, M.P., 2010. Fundamentals of modern manufacturing: materials, processes, and systems. John Wiley & Sons.
6. Rao, P.N., Manufacturing Technology Foundry, Forming and Welding, 2008.

These are the references which we have used for preparing this slide. Thank you very much.