

Basics of Materials Engineering
Prof. Ratna Kumar Annabattula
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture - 03
Crystal Structure - 1 (Platonic Solids)

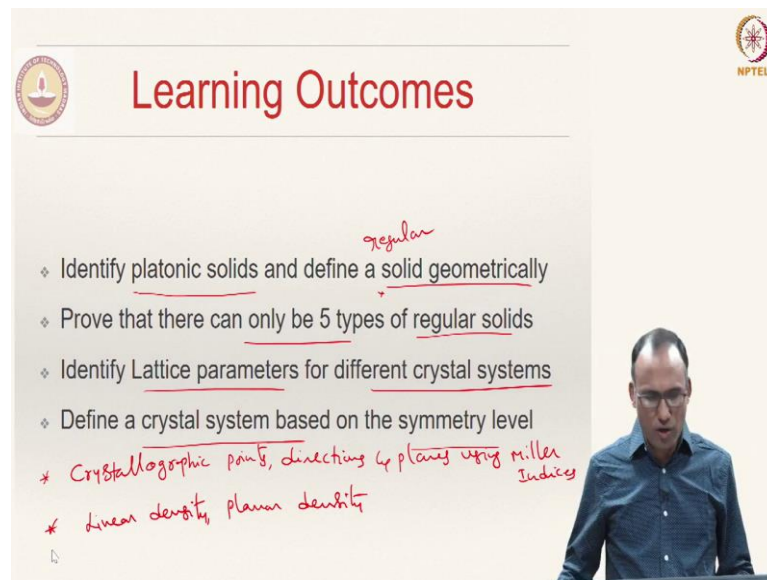
So, welcome back. In the last class we have looked at the material property landscape, and then we have discussed how the structure of the material gives rise to certain properties. And that in turn, determines the performance of a component, right?

(Refer Slide Time: 00:29)



So, in this class we will look at the structure of materials, particularly at the atomic scale. And then, towards the end of this module we will see how the structure gives rise to certain properties.

(Refer Slide Time: 00:45)





The slide is titled "Learning Outcomes" and features a list of four bullet points. The first bullet point is "Identify platonic solids and define a solid geometrically", with the word "regular" written in red above "solid". The second bullet point is "Prove that there can only be 5 types of regular solids". The third bullet point is "Identify Lattice parameters for different crystal systems". The fourth bullet point is "Define a crystal system based on the symmetry level". Below the list, there are two handwritten notes in red: "* Crystallographic points, directions & planes using miller Indices" and "* linear density, planar density". The slide also includes logos for IIT Bombay and NPTEL.

So, the learning outcomes of this module or -- so we should be able to identify -- we will define something called Platonic solids. And we should be able to identify these Platonic solids and define a solid geometrically. What is the definition of a solid geometrically, or rather a regular solid? And we will prove that there can only be 5 types of regular solids.

And then, we should be able to identify lattice parameters for different crystal systems, and define a crystal system based on the symmetry level. So, these are the 4 learning outcomes. And then we should also be able to define something called crystallographic points, directions, and planes, using miller indices. And then we will also talk about something called linear density, planar density.


And towards the end, we will talk about the theoretical density of a material. So, these are our learning outcomes.

(Refer Slide Time: 02:07)



Structure (from sub atomic to atomic)

- ❖ Interatomic bonding is determined by the electron structures of individual atoms
- ❖ Reading assignment: Callister's Chapter 2 (Atomic Structure and Interatomic Bonding)
- ❖ Today, we will discuss the structure at atomic level, i.e., arrangement of atoms in solid state



So, before we can actually start talking about structure -- when we are talking about structure in this module we are actually going to talk about structure at the atomic scale. So, how the atoms are arranged in a solid material, and we are restricting our ourselves to the study of materials in the solid state, ok? So, when we are talking about structure, it actually can span from subatomic structure to the macroscopic structure, right?

So, but here this module concerns up to the structure at the atomic scale. But before atomic scale can be studied, it is instructive to also have some idea or some knowledge about the structure at the subatomic scale, which determines how the bonding between individual atoms takes place in a material, right? So, the module on interatomic bonding will not be discussed in this class. Because this topic has been dealt in detail probably in your plus 2 or earlier.

So, we expect that you should be able to revise the concepts of interatomic bonding on your own. And the relevant textbook which you might want to look at in order to understand the interatomic bonding and the structure of atoms is Callister's Material Science and Engineering textbook, Chapter 2, which talks about atomic structure and interatomic bonding. And so, having said that, we assume the knowledge of this interatomic bonding in order to continue these lectures on crystal structure, ok?

So, we are going to talk about structure at atomic level, that is the arrangement of atoms in a solid state.

(Refer Slide Time: 03:50)

Platonic Solids

- ❖ Tetrahedron
- ❖ Hexahedron
- ❖ Octahedron
- ❖ Dodecahedron
- ❖ Icosahedron

Regular Convex Polyhedra

Alright, so to begin with, we will talk about something called Platonic solids. So, the solids which are called regular solids are classified into five categories known as Platonic solids. They are named after Greek philosopher Plato, and these are also known as regular convex polyhedral, ok?

(Refer Slide Time: 04:20)

Platonic Solids

- ❖ Tetrahedron ⁴
- ❖ Hexahedron ⁶
- ❖ Octahedron ⁸
- ❖ Dodecahedron ¹²
- ❖ Icosahedron ²⁰

So, these five of them are named as tetrahedron, hexahedron, octahedron, dodecahedron, icosahedron. So, tet actually means 4, hex means 6, oct means 8, dodeca means 12, icosahedron means 20, right? So, here, what is 4?

4 is nothing but you have 4 faces to this particular polyhedron, here you have 6 faces that is why it is hexahedron, octahedron, dodecahedron and icosahedron, right? So, I am sorry, so this should be 20 faces not 21. So, icosahedron has 20 faces.

(Refer Slide Time: 05:14)

The slide is titled "Platonic Solids" and features a list of five solids with their respective face counts and associated names. The solids are represented by red 3D models. The list is as follows:

Solid	Number of Faces	Associated Name
Tetrahedron	4	Pythagoras
Hexahedron	6	Pythagoras
Octahedron	8	Theaetetus
Dodecahedron	12	Pythagoras
Icosahedron	20	Theaetetus

At the bottom of the slide, there is a link for more information: https://en.wikipedia.org/wiki/Platonic_solid. A small inset image of a man in a blue shirt is visible in the bottom right corner of the slide.

Okay, let us see why there should only be these 5 solids, why cannot we have more than this number, ok? So, as I have discussed tetrahedron has 4 faces, hexahedron has 6 faces, octahedron has 8 faces, and so on. These type of solids were known before Plato.

But Plato was the one who actually summarized all of them and then wrote an article about them. And hence, in his honor, these solids are named after him. But there are individuals who are responsible for identifying each of these solids, like for instance tetrahedron was due to Pythagoras, and so on right?

(Refer Slide Time: 05:59)

The slide is titled "Platonic Solids" in red text. It features a list of five solids on the left, each with a red checkmark and a corresponding 3D model on the right. The solids are: Tetrahedron, Hexahedron, Octahedron, Dodecahedron, and Icosahedron. The Dodecahedron and Icosahedron entries include the text "quasi crystals, bucky balls" below them. A red circle highlights the word "Dodecahedron" in the list. In the center of the slide is a painting of Plato and Aristotle. Below the painting, the text reads "Plato (left) with his student Aristotle (right)" and "Source: wikipedia". At the bottom left, there is a source attribution: "Source: Robert Webb's Stella software <http://www.software3d.com/Stella.php>". The NPTEL logo is in the top right corner.

- ❖ Tetrahedron ✓
- ❖ Hexahedron ✓
- ❖ Octahedron
- ❖ Dodecahedron ✓
quasi crystals, bucky balls
- ❖ Icosahedron ✓
quasi crystals, bucky balls

Plato (left) with his student Aristotle (right)
Source: wikipedia

Source: Robert Webb's Stella software <http://www.software3d.com/Stella.php>

And so, the structure of tetrahedron and hexahedron is probably known to us very well: most of the crystalline materials as we will see later in the course. But the last two structures i.e., the dodecahedron and the icosahedron, were not observed in real materials or solid materials until very recently, until people actually discovered a new class of materials called quasi crystals, which seems to show this crystal structure comprising of dodecahedron and icosahedron structures i.e., both quasi crystals and bucky balls, ok?

So, here we are showing Plato on left hand and with his student Aristotle. Aristotle also is one of the famous Greek philosophers who we are familiar with as well alright.

(Refer Slide Time: 06:53)

Platonic Solids (Pancha Boothas)

- ❖ Tetrahedron Fire
- ❖ Hexahedron Earth
- ❖ Octahedron Air
- ❖ Dodecahedron Sky (Ether)
- ❖ Icosahedron Water

quasi crystals, bucky balls

Source: Robert Webb's Stella software <http://www.software3d.com/Stella.php>

Alright. So, these Platonic solids are also connected, so there are five of them. In Indian mythology we believe that the entire world is made of Pancha Boothas, right?

So, in a corollary people have historically connected these five Platonic solids with the five elements like fire, earth, air, ether or sky and water, right? It is only a philosophical connection just to say that only these five of them will make the entire universe.

(Refer Slide Time: 07:33)

What is a regular solid ?

- ❖ A regular solid is formed when more than two regular polygons meet at a corner and the total internal angle at the corner is less than 360°

<http://www.mathsisfun.com/geometry/platonic-solids-why-five.html>

So, before we actually prove that the regular solids or Platonic solids can only be five, you cannot have more than 5 regular solids, we should first understand the definition of a regular solid. What do we mean by a regular solid?

So, a regular solid is formed when more than two regular polygons meet at a corner. So, at a corner at least three regular polygons should meet. More than two means at least three regular polygons should meet at a point. And the total internal angle at the corner should be less than 360 degrees.

For instance, if we take this cube you have the internal angle here 90 degrees, 90 degrees, 90 degrees. The sum of these angle should be less than 360. If it is less than 360 only then it will become a solid, otherwise if it becomes 360 then it will become a flat plane. So, that is why it should be less than 360 degrees.

So, the Platonic solid is actually made of these regular polygons meeting at a point, but each and every point within this Platonic solid will have same number of these regular polygons meeting.

(Refer Slide Time: 08:49)

How many types of regular solids are possible?

Geometry	Number	Total angle	Solid
Triangle (60°)	3	180	Tetrahedron
	4	240	Octahedron
	5	300	Icosahedron
Square (90°)	3	270	Hexahedron (cube)
	4	360	X
Pentagon (108°)	3	324	Dodecahedron
	4	432	X

Source: Robert Webb's Stella software <http://www.software3d.com/Stella.php>

So, now, let us look at how many types of these regular solids possible. So, let us look at the geometry. If you take triangle, regular triangle means it is a triangle with all the sides equal, and all angles will be 60 degrees. So, how many of them should meet according to

the definition of a regular solid? More than two, that means, at least 3 should meet at a point. If 3 triangles meet at a point the total angle will be 3 times 60 i.e., 180 degrees.

So, that is what is going to be our tetrahedron. You can see that at this point 1, 2 and there is another one on that side. So, 3 triangles are meeting, and all of them are equilateral triangles, ok? So, only then it is called a regular solid. And suppose if 4 of them meet -- 4 triangles meeting at a point -- four 60's is 240 -- still less than 360, and hence that will be your octahedron. So, at a point you have 4 of them meeting 1, 2, 3 and 4, right? So that will be our octahedron.

If 5 of them are meeting, 360 -- five 60's are 300, so that will give us our icosahedron with 20 faces. 1, 2, 3, 4, 5; 5 of them are meeting at this point, right? And then, let us say next you can have 6 of them meeting. 6 of them meet then it will give 360 degree; that means, it is equal to 360 and hence it does not qualify as a regular solid. So, with the triangles, you can have these 3 combinations. Now the next polygon after triangle is the square.

So, where the angle is 90 degrees. So, 3 of them meeting will give you 270, and that will be our hexahedron. But if 4 squares meet at a point then that becomes 360, then it cannot be a regular solid. So, with square as a face you can only have 1, that is hexahedron.

Now, let us talk about pentagons -- 3 of them -- three 108's is 324, and that is our dodecahedron, right? And if you take 4 of the pentagons, that is going to be more than 360 then -- and hence it will not be possible. And let us take hexagon -- 3 of them will meet -- then 3 into 120 will be 360, and hence it cannot be a regular solid.

So, any other higher dimensional geometry will not give you the total included angle less than 360. And hence, we can clearly see that there are only 5 types of regular solids that are possible, and these 5 solids are called Platonic solids.

(Refer Slide Time: 11:38)

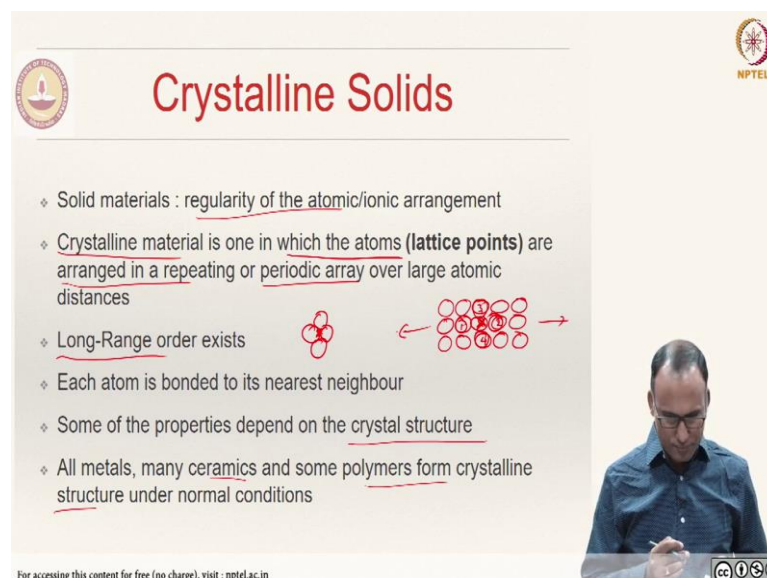


The slide features a title "How about a Hexagon?" in red. It includes two bullet points: "Hexagon's internal angle is 120° and hence 3 times 120 is 360° . Hence, it can't be a solid, but a tiling." and "How is a soccer/volley ball made? (Hexagons?)". A small image of a soccer ball is shown below the text. The NPTEL logo is in the top right corner, and a speaker is visible in the bottom right corner.

So, how about hexagon? As I have mentioned hexagons internal angle is 120° and hence 3 times 120° , 360° hence it cannot be a solid, but a tiling. But have you ever seen a soccer ball? So how is the soccer ball made? Is it completely made of hexagons?

Let us look at it. So here this is 1 hexagon. 1, 2 but the third one meeting at this corner is not a hexagon, this is a pentagon. So, you cannot simply make a solid out of regular hexagons, right? Here you have a pentagon. So, only 2 hexagons are meeting then it is not becoming a regular solid because all the faces are not the same, it cannot be made.

(Refer Slide Time: 12:21)



The slide features a title "Crystalline Solids" in red. It includes several bullet points: "Solid materials : regularity of the atomic/ionic arrangement", "Crystalline material is one in which the atoms (**lattice points**) are arranged in a repeating or periodic array over large atomic distances", "Long-Range order exists" (with a diagram of a small cluster of atoms), "Each atom is bonded to its nearest neighbour", "Some of the properties depend on the crystal structure", and "All metals, many ceramics and some polymers form crystalline structure under normal conditions" (with a diagram of a larger crystal lattice). The NPTEL logo is in the top right corner, and a speaker is visible in the bottom right corner.

So, having discussed the basic classification of these solids into Platonic solids, we will see in our discussion there are crystal structures which will use one of them as the underlying elements for our crystal structure, ok?

So, what are these crystalline solids? And here in this class we are only going to talk about crystalline materials not amorphous materials. What do we mean by a crystalline material and amorphous materials, we will talk about it.

So, solid materials are characterized by the regularity of the atom or ionic arrangement. And a crystalline material is one in which the atoms are arranged in repeating or periodic array over long atomic distances. That means, in a crystalline solid material, the atom should be arranged in a periodic manner, such that the structure at any point within the material should look exactly the same.

That means, for instance if my atoms are arranged like this -- assume all of them are of same size. If I am standing here then I am seeing 1, 2, 3, 4 -- these are my nearest neighbors, because this guy is farther than this guy. So, imagine they are touching each other. And if I move in this direction, and in this direction, let us say I moved 10 kilometers if it is a crystalline material. And if I stand at any point, I should again find 4 nearest neighbors.

Suppose if I am standing here and imagine myself as an atom and then I will be pulled by the surrounding atoms because of the inter-atomic bonding. So, the amount of force that I am experiencing by sitting at this cross position or standing at the cross position -- that means, the force field that I am experiencing at this position should not change if I move far away from this point and stand at another position. And I should experience exactly the same force field that is what we mean by long-range order.

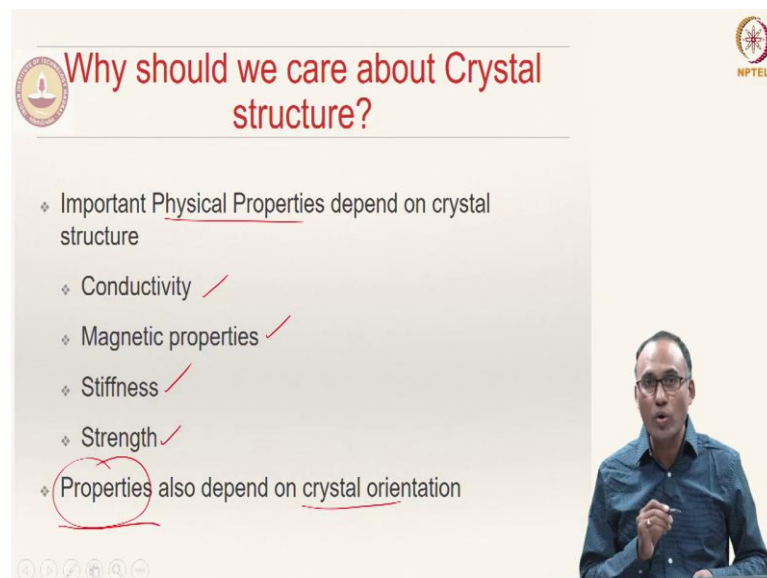
That means we should not be able to distinguish this point or this point in terms of the force fields or the atomic arrangements. And if the atoms are arranged in such a manner, such a system is called a crystalline system.

The key here is that the long-range order should exist. The order should be existing over a long range, it should not be only local. If it is locally having certain order, but far away it does not have that order, then such a material cannot be called as a crystalline material.

Crystalline material by definition is actually a material which has some order to it. And a material which does not have such an order is called an amorphous material or non-crystalline material. In this class, we are only going to talk about crystalline materials. Some of the properties of the materials that we are going to talk about actually depend on the structure or the crystal structure.

How the atoms are arranged is going to determine the properties of these materials. All metals, many ceramics and some polymers form crystalline structure under normal conditions, right? And normally they will form crystalline structure, but you can also do additional process to actually make amorphous forms of them. In general, most of the metals are crystalline in nature.

(Refer Slide Time: 16:11)



The slide features a title "Why should we care about Crystal structure?" in red text. Below the title is a list of properties: "Important Physical Properties depend on crystal structure", "Conductivity ✓", "Magnetic properties ✓", "Stiffness ✓", "Strength ✓", and "Properties also depend on crystal orientation". The word "Properties" in the last item is circled in red. The slide includes a logo on the top left, an NPTEL logo on the top right, and a small video inset of a man speaking in the bottom right corner.

So, why should we care about the crystal structure? We should care about crystal structure because important physical properties of materials depend on crystal structure. What are these important physical properties? Thermal or electrical conductivity, magnetic properties of the material, mechanical stiffness of the material or the tensile strength of the material. These guys depend on the crystal structure of the material.

And in addition, it is not just the crystal structure that is important. The property is actually the response to the external stimulus, right? We have already discussed. What do we mean by a property? Property of a material is the characteristic response of the

material to the external stimulus. So, the direction of the external stimulus with respect to the crystal orientation is also going to determine the properties.

So, the properties depend not only on the crystal structure, the relative orientation of the external stimulus with respect to the crystal structure is also going to change the properties of the material. So, they also depend on the crystal orientation.

(Refer Slide Time: 17:20)

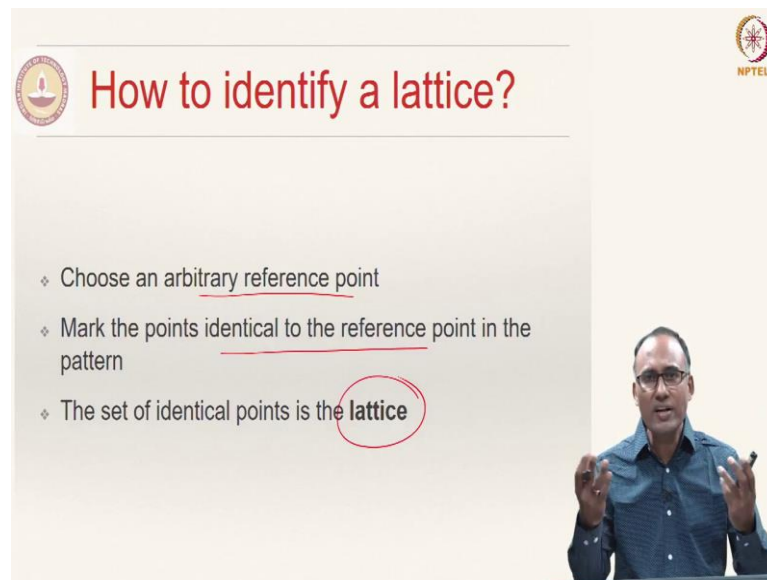
The slide is titled "Crystalline Structure" in red text. It features a list of characteristics on the left side, each preceded by a diamond symbol (❖). The list includes: "Characterised by repeating structures in three dimensions", "Lattice", "Lattice Points", and "Unit Cell". Red handwritten marks are present: three slashes next to "Lattice", a bracket grouping "Lattice Points" and "Unit Cell", and two slashes next to "Unit Cell". In the bottom right corner, there is a small inset video of a man in a blue shirt looking at a laptop. The slide also contains logos for IIT Bombay and NPTEL.

- ❖ Characterised by repeating structures in three dimensions
- ❖ Lattice
- ❖ Lattice Points
- ❖ Unit Cell

We have discussed about this long-range order, but how do we characterize this long-range order or the repeating structures in 3D. They are characterized by the concepts called lattice or lattice points or unit cells.

So, we should understand these three concepts in order to be able to say something or characterize the repeating structures in 3 dimensions.

(Refer Slide Time: 17:41)



The slide features a title "How to identify a lattice?" in red text at the top. Below the title are three bullet points, each starting with a diamond symbol. The first bullet point is "Choose an arbitrary reference point". The second is "Mark the points identical to the reference point in the pattern". The third is "The set of identical points is the **lattice**", where the word "lattice" is circled in red. In the bottom right corner, there is a small inset image of a man in a blue shirt and glasses, gesturing with his hands as if presenting.

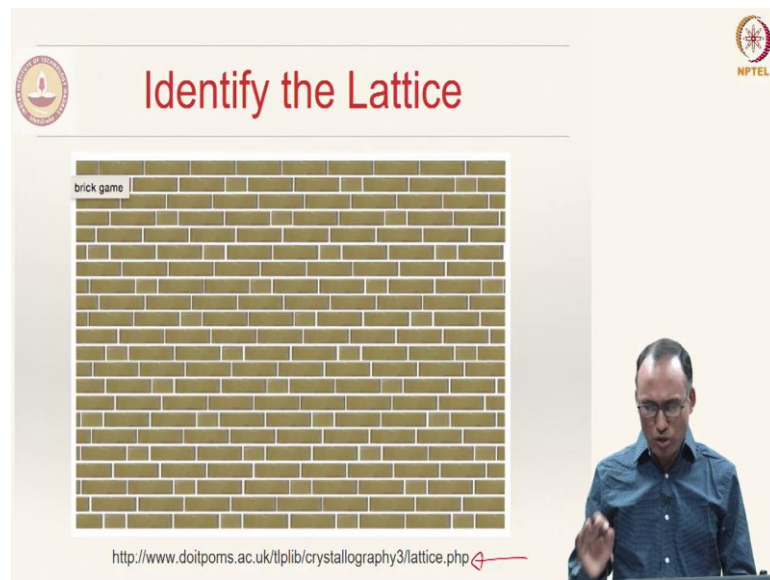
- ❖ Choose an arbitrary reference point
- ❖ Mark the points identical to the reference point in the pattern
- ❖ The set of identical points is the **lattice**

So, and then the question is, how do we identify a lattice? How to identify a lattice of a crystal structure? What do we mean by lattice in the first place? So, if you are given a material or if you are given a system, in order to identify a lattice all that you need to do is you first choose an arbitrary reference point. It can be any point within the system. Choose some reference point arbitrarily.

And now, you look at the point and identify its characteristics, and then, start identifying or start marking points which are identical to the reference point in the system, right? You will choose any point as a reference point and I start identifying all the points elsewhere in the material which are identical to this reference point. And the set of all such identical points is what we call lattice.

The definition of lattice is basically the set of identical points that you can find in a system.

(Refer Slide Time: 18:41)

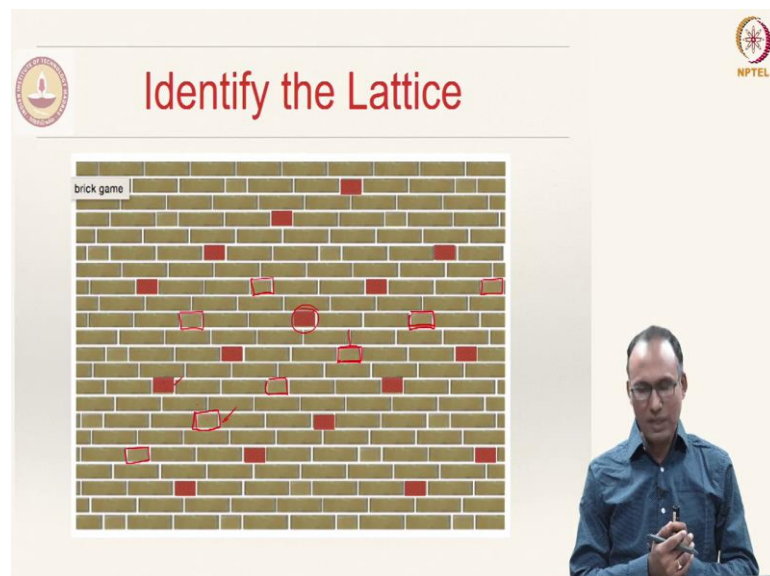


The slide features a title "Identify the Lattice" in red text at the top center. On the left, there is a circular logo with a lamp. On the right, there is an NPTEL logo. The main content is a photograph of a brick wall with the text "brick game" in the top left corner. Below the wall, a URL is provided: <http://www.doitpoms.ac.uk/tlplib/crystallography3/lattice.php>. A red arrow points to the end of the URL. In the bottom right corner, a man in a blue shirt and glasses is speaking.

I have taken this picture from Cambridge material science course on crystallography. The details about this crystal lattice and lattice structure can be found at this particular web resource. I encourage all of you to go through this web resource which gives you a better understanding of what we are discussing in this class.

So, this is a wall, a brick wall, right? So, let us look at the pattern that is available in this brick wall, and let us try to identify the lattice. What is the guideline for identifying a lattice? First, we need to choose a reference point.

(Refer Slide Time: 19:28)



The slide features a title "Identify the Lattice" in red text at the top center. On the left, there is a circular logo with a lamp. On the right, there is an NPTEL logo. The main content is a photograph of a brick wall with the text "brick game" in the top left corner. Several red squares and circles are overlaid on the wall, highlighting specific points. In the bottom right corner, a man in a blue shirt and glasses is speaking.

So, let us choose that as a reference point. And now, having chosen this as a reference point, now we need to identify all the identical points. So, what are the other identical points?

So, we can see these are our identical points, right? So, now, you remove the background pattern.

(Refer Slide Time: 19:58)



These are the set of points that you are left with and this is what we call lattice of the underlying structure. Your lattice could have been different if you have chosen some other point as a reference point. Suppose if you have chosen instead of this as your reference point, if you have chosen this as your reference point, then your lattice would have been -- identical points right? -- so, this is 1, this is 2nd one, and 3rd one, 4th one, 5th one, 6th one.

So, these two are not the same, please note that. Here, below this there are two whereas, above this there are two. So, you have to be careful in identifying. Similarly, this is another lattice point, and that is another lattice point identical to this. So, one would be able to obtain depending upon the choice of the initial reference point your crystal lattice could be different. But the point is that you will be able to get back the original structure if you carefully look at the lattice.

(Refer Slide Time: 21:01)

Unit cell

- ❖ Repeated elements (**unit cells**) in three dimensions
- ❖ Unit cells are the building blocks of crystal structure
- ❖ **Primitive and non-primitive unit cells**
 - ❖ Primitive: only one lattice point per unit cell
 - ❖ non-primitive: more than one lattice point per unit cell

http://www.doitpoms.ac.uk/tlplib/crystallography3/unit_cell.php

The points are called lattice points and the collection of these points is what we call lattice. Next, we will discuss what we mean by unit cell. A unit cell is nothing but a repeated set of elements in 3D. Unit cells are the building blocks of our crystal structure. They are the building blocks of our crystal structure. If you take a unit cell and then span them in 3D in all the 3 directions, you will get a crystal.

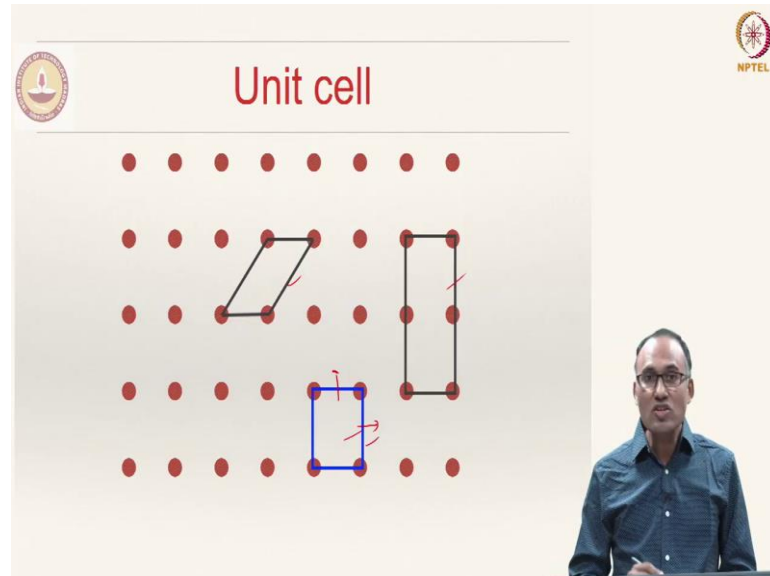
The unit cells are classified into two primary types; one is primitive unit cell and non-primitive unit cell. What do we mean by primitive unit cell? A primitive unit cell is the one which has effectively only one lattice point per unit cell and non-primitive unit cell can have more than one lattice point per unit cell. For instance, if we take this lattice, you can identify this parallelogram as one of the unit cells. If you span this unit cell in 2D, then you will be able to fill the space.

So, now why do you say that it is effectively one unit cell i.e., one atom per unit cell? There is another unit cell here, another unit cell here, another unit cell here, and another unit cell here. Now, if you take this point, this atom is shared by four unit cells. So, effectively only one-fourth of this atom is part of this unit cell. One-fourth of each corner atom is actually belonging to this unit cell.

So, there are four corner atoms and effectively one atom per unit cell. If you take this guy -- 4 corner atoms -- one-fourth of them each, but there is a central atom. So,

effectively you have two atoms per unit cell, and such a unit cell is called non-primitive unit cell.

(Refer Slide Time: 23:19)



Let us say you have this lattice. So, you have identical points which are spanning in all the two directions. We are only looking at two dimensional lattices. Now, how do we identify unit cells? These are all valid unit cells.

What do the mean by valid unit cell? If you can translate this unit cell in both x and y directions, by an amount equal to interatomic distance, then you will be able to fill the entire space without leaving any voids behind. And that is how you should identify a unit cell, right?

So, this is one possible unit cell, this is another possible unit cell, this is another possible unit cell. However, this is the smallest unit cell.

(Refer Slide Time: 24:14)

Unit cell

- All the parallelograms are valid unit cells
- Square is the smallest with most symmetry

The square is the smallest unit cell, and in general all parallelograms are valid unit cells in 2D, and all the parallelepipeds are valid unit cells in 3D. The square is the smallest with most symmetry. The level of symmetry is highest for square compared to these unit cells.

(Refer Slide Time: 24:35)

Unit Cell

- Smallest unit cell might not reflect symmetry
- Larger unit cell is chosen
- Primitive or non-primitive

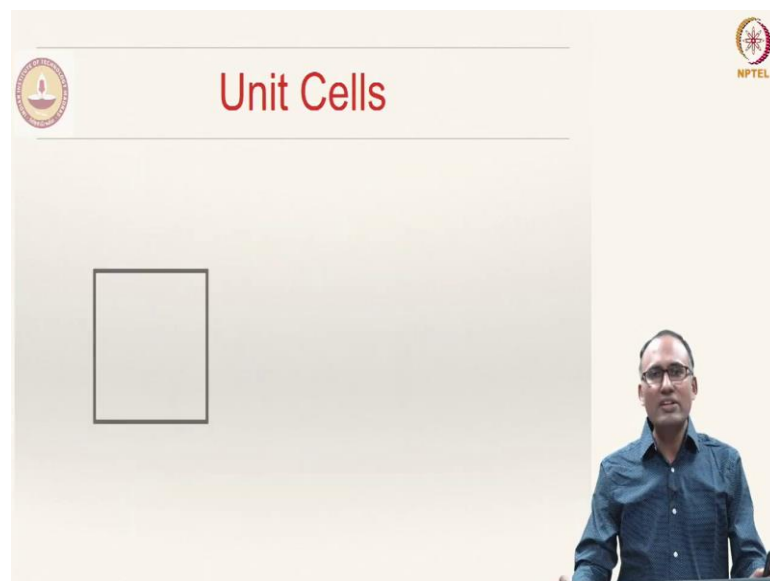
You can also for instance have another structure, wherein you cannot identify a square as a unit cell. So, you see that this is one unit cell, this is another unit cell. So, the smallest

unit cell might not reflect the symmetry of the crystal structure, and you might choose the larger unit cell as the primary unit cell. It can be primitive or non-primitive.

That means, whenever you are choosing a unit cell, it does not have to be the smallest, but choosing the smallest one is usually the convention. Sometimes the smallest unit cell might not reflect the symmetry of the crystal. So, here this is the smallest unit cell, but the symmetry level is higher for this unit cell. Hence, you might want to choose this as your unit cell, but in principle you can choose any one of them. You can actually define more than one unit cell.

You could have this, or you could also have another unit cell. For instance, this could be another unit cell, and this could be another unit cell, and so on. These are all possible. So, in principle you should be able to find several valid geometries that are parallelograms in 2D, as unit cells.

(Refer Slide Time: 25:59)



With that I will close this module. And then we will discuss more details on the unit cells, and what do we mean by a crystal, how do we differentiate a crystal and a lattice, and so on in the next class.

Thank you very much.