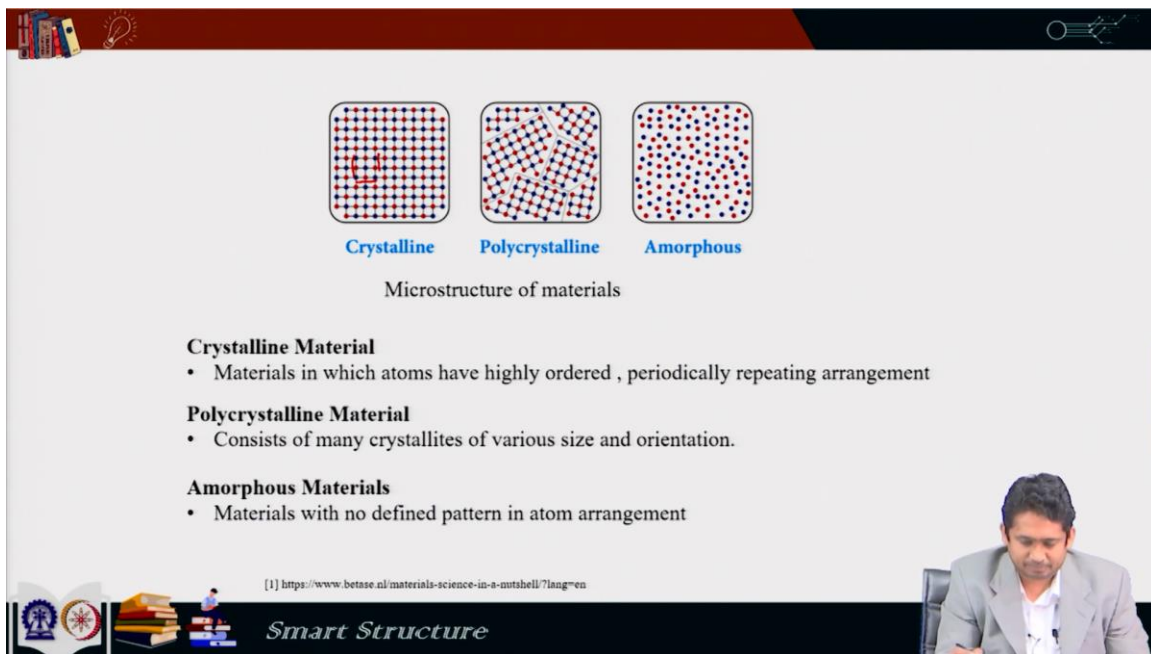


Smart Structures
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Week 01
Lecture No: 04
Introduction to Piezoelectric Materials
Part 01

Welcome to the third lecture.

Now, we will start talking about Piezoelectric Materials.

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Crystalline **Polycrystalline** **Amorphous**

Microstructure of materials

Crystalline Material

- Materials in which atoms have highly ordered , periodically repeating arrangement

Polycrystalline Material

- Consists of many crystallites of various size and orientation.

Amorphous Materials

- Materials with no defined pattern in atom arrangement

[1] <https://www.betase.nl/materials-science-in-a-mutshell/?lang=en>

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Now, to understand this piezoelectric materials or piezoelectricity, we need to first understand crystalline and polycrystalline materials and some of the concepts of symmetry. Crystalline materials are materials where atoms have highly ordered periodical repeating arrangements. For example, if we see here we can see that if we just take maybe this unit, we can see that this unit keeps repeating. So, if we go in this direction, if I go down below, if I go diagonally, I can see this pattern keeps repeating.

So, it is a crystalline material. At the other end of it is an amorphous material. In amorphous material, there is no periodic pattern. So, we can see it here.

We cannot define a something which repeats here. Polycrystalline materials is something which can be thought to be in between these two because here, in a global sense, there is no repeating pattern, but within each domain. We can see that there is something which

repeats. For example, here we can see that this cell keeps repeating, same thing we can see here, but if I compare these two domains or these two domains, we can see that the orientations are different. So, within each domain, these units have their own orientation and that remains consistent, but in two domains, the orientation may not match. So, that is why it is called a polycrystalline material.

Now comes symmetry. So, we have three elements of symmetry, one is plane of symmetry, axis of symmetry, and center of symmetry. Now, a plane of symmetry is if an imaginary plane can divide the crystal into two parts, which are mirror images of each other. Then, we call it a plane of symmetry. For example, if we have something like this, if we think of one plane here. So, this plane at the middle divides it into two halves, and these two halves are mirror images of each other.

Similarly, we can draw another plane here also and divide it into two equal parts. So, these are all planes of symmetry, and these are generally called rectangular planes of symmetry. Now, there can be for the same cube, we can think of a plane like this which goes diagonally and that also divides it into two parts which are mirror images of each other. So, that becomes a diagonal plane of symmetry.

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Crystal Symmetry

Plane of symmetry

Axis of symmetry

Centre of symmetry

Plane of symmetry

- If an imaginary plane can divide the crystal into two parts which are mirror images of each other, that plane is plane of symmetry.

Rectangular planes of symmetry

Diagonal plane of symmetry

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Similarly, there can be an axis of symmetry. So, it is an imaginary axis about which, if the object is rotated, its appearance is repeated more than once. Now, something which does not have an axis of symmetry it needs to be rotated by 360 degrees for the same shape to come. So, that is why we do not consider that, but where it appears more than once, then we can say that it has an axis of symmetry. So, in 360 degree rotation, if the appearance

comes n times, then it calls an n -fold symmetry, which means the appearance occurs after a rotation of 360 degrees by n . For example, here we have something called two-fold axis or diad. So, here, the appearance comes after 180 degree rotation.

Now, to understand this, let us name them. Maybe we can call it one two three four five six seven and eight. So, if it rotates by an angle 180 degrees, let us imagine that these are the hidden lines. So, what is visible to us is this line one two three four, this face one two three four. So, if it rotates by an angle 180 degree, then what we can see here is this.

So, we have after rotation, the face that comes is seven six five eight and three two one four. So, the other face five six seven eight that comes in the front and one two three four goes back, which means the this, this, I mean this shape again reappears. So, it is a two-fold axis of symmetry. In a three-fold axis, the axis connects this corner with this corner. So, if it is rotated an angle 120 degrees, again, the same face comes.

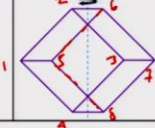
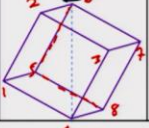
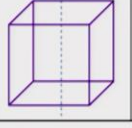
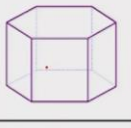
If you want to understand it, let us again name it one two three four, and let us assume that these two lines are hidden lines. So, we see the one two three four face from the front, and then we have five six seven eight. So, if it rotates by an angle 120 degrees, then what we see is this. In that case, this face, which is three seven eight four that comes here, and accordingly, the other points take place. So, after 120 degree rotation, the shape again comes back. So, that is why it is a three-fold axis or triad.

Four-fold axis, it is easy to visualize if it is just given a 90 degree rotation, this face comes here, and that is a four-fold axis or triad. And then six-fold axis again if it is given a 60 degree rotation, this face comes here and accordingly the other face takes their shape. So, the shape repeats at an angles or after rotation of angle 60 degree. So, it is a six-fold axis or hexade.


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Axis of symmetry

- It is an imaginary axis about which if the object is rotated, its appearance is repeated more than once.

Axis	Two fold axis or diad:	three fold axis or triad axis	Four fold axis or tetrad axis	Six fold axis or hex ad axis
Similar Appearance After Rotation	180°	120°	90°	60°
Figure				

Handwritten diagrams below the table show a cube with red numbers 1-8 at its vertices and a vertical axis of symmetry passing through the center.



Now, we will talk about center of symmetry. Now, center of symmetry, if there is a point inside the line through which the line drawn through which touches the surface of the crystal at an equal distance in two opposite directions, then that point is called a center of symmetry. Again, if I take the example of this of a cube. So, let us imagine that the, let us imagine the coordinates to be zero zero zero, one zero zero and we have one one zero, we have zero one zero here and then we have one one one, one zero one, zero zero one, and we have zero one one. Now, let us imagine one point at the center P and P suppose it is half, half, half. So, if I draw a line vertical line through P, it touches the top surface here, and it touches the bottom surface here.

Now, the distance of this point from P is same as distance at this point from P. Similarly, if I draw a line here, a horizontal line, it touches the right face, it touches the right face here, and it touches the left face here, and again the distance of this point from P and this point from P is same. We can do the same thing through diagonals also; if I draw a line, from this and from here, again, it touches the two corners at the two, at two equal distances. So, the point P is center of symmetry for this object, and only one center of symmetry can exist.

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Centre of symmetry

- A point inside, line drawn through which touches the surface of the crystal at equal distance in two opposite directions.
- Only one centre of symmetry can exist

$P \equiv \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

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Now, we will talk about symmetry operations. So, symmetry operations are something which, after being carried out, leaves the object looking same, and there are various types of symmetry operations. The first one is translation symmetry. So, let us imagine that we have objects like this. It can be in 3D. So, we are drawing it in 2D for the sake of easiness. So, let us assume that we have a 2D array kind of structure. It can go in this direction, it can go in this direction, it can go, it can go.

Now, here, the distance between these two successive objects are same. So, it is all say a , it is all a . So, they are not changing; although in the drawing, it may not be accurate and look little different, but they are all same. Similarly, in the vertical dimension, let us say they are all b . Now, if I take a point here and if I look around. So, it says point one. So, if I take a point here and if I look around. So, whatever I see, if I take a point here also and if I look around, I would see the same thing also, or in other words, if I take this point and replace and put it here, the look does not change. So, after translation, it remains invariant, but here we have to understand that this translation has to be at a distance, which is integer multiple of this a and b . So, if you are shifting towards this axis, the horizontal axis, it has to go a , two a , three a , like that in the vertical direction. It has to go b , two b , three b like that. So, if I do that kind of translation, it looks same. So that is why it is called a translation symmetry.

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Symmetry Operations
 An operation which after being carried out leaves object looking the same

1. Translational Symmetry Operation

The diagram shows a 2D lattice of red dots. A central dot is labeled '1'. A horizontal dashed line passes through the center. To the left, a vertical line is marked with 'b' and four tick marks. Below the grid, a horizontal line is marked with 'a' and four tick marks.


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Reflection symmetry. A plane or line that divides the crystal into two equal parts, which are mirror images of each other. Again, we can look into the circle. We can see that we have a line here that divides the circle into two equal parts, not just equal and I mean, similarly looking parts, which are mirror images of each other, and it also divides it into two mirror images, and we can think of a lot of axes, I mean an infinite number of axis for this circle which can divide it into two equal parts. Rotation symmetry. So, here, rotation by an angle θ gives the same crystal. We have already seen; we have already seen that there is an axis of symmetry with respect to which we rotate; we get the same shape back. So, if we do that operation, we get a rotational symmetry operation. Then, inversion symmetry. Again, if for every lattice point at r , there exists a lattice point minus r , and it is applicable to 3D only. We have also seen this.

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2. Reflection Symmetry Operation

- A plane or line divides the crystal into two equal parts which are mirror images of each other.

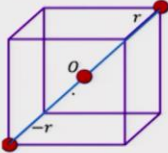


3. Rotation symmetry

- Rotation by an angle θ gives the same crystal

4. Inversion Symmetry

- If for every lattice point at r , there exists a lattice point at $-r$
- Applicable only for 3D



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Now, there is something called Rotoinversion. Rotoinversion means if the object comes back after a rotation and the inversion, then we can call it a Rotoinversion. For example, let us imagine this. Let us imagine that we have one atom here and here, and they are same. So, if this is rotated by an angle 360 degrees, it comes back here. If this is rotated by an angle 360 degrees, it comes back here. So, we are doing a one-fold rotation to both, and then if they interchange their points.

So, the center is somewhere here. So, with respect to this, if this point comes here and this and this point goes here, which means the interchange their point and their locations, these two points interchange their locations, then what we get is point two here and point one here, and even then, it looks same. So, after a rotation by 360 degrees and then inversion, we get the same shape back.

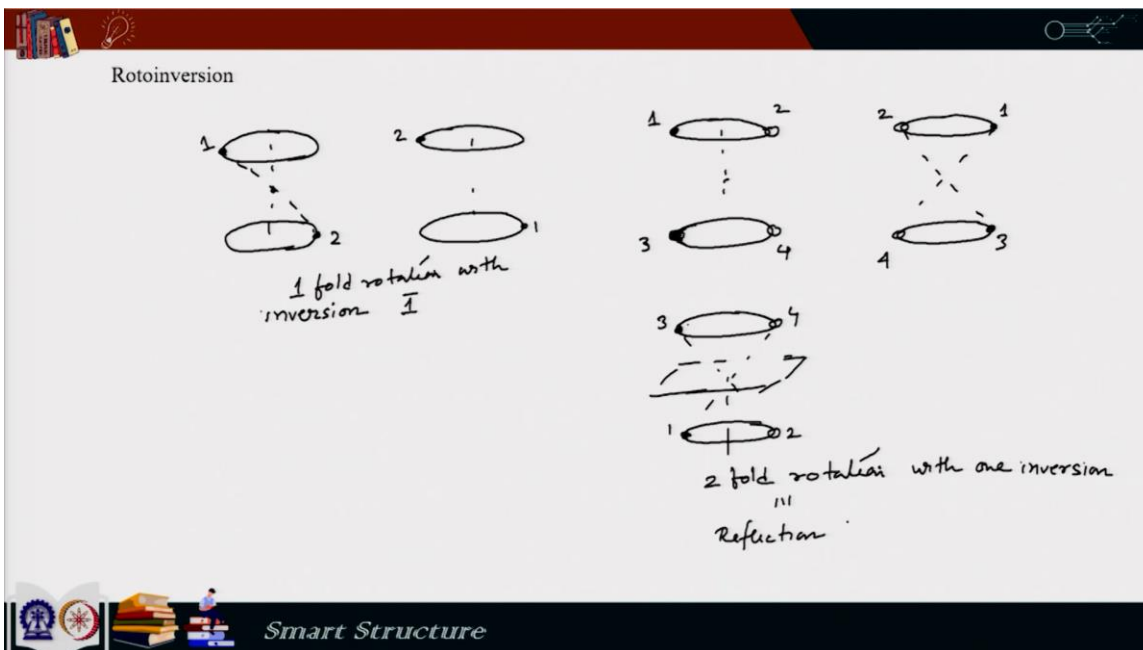
So, it is a one-fold rotation with inversion. So, we denote it by one bar. Now, the point to note is that here we rotated this by 360 degrees, which means that is not a proper rotation because it is not needed actually; without even rotating also, we could have just interchange the place and get it.

Now comes two-fold symmetry with two-fold rotoinversion, that means two-fold rotation with inversion. To understand this, let us imagine a situation like this: suppose we have an atom here, and we have something here, but these two are different. So, that is why they are one is solid, one is hollow, and then we have three here, and we have, we have it here four. Now, if they interchange their place, then four will go here, one will come here, which means the shape does not remain same. So, what has to be done here is before doing the inversion, it has to be rotated. So, if it is rotated by an angle 180 degrees, then, then two comes here, and one goes here, and similarly, if the bottom part is also rotated by 180

degrees, then three comes here, and four comes here. Now, if they interchange their location so, which is, which can be seen here, then what we see is three sitting here, and four sitting here, and we see one coming here and two coming here, which means again we get our previous shape back. So, it is possible through one 180 degree rotation and then one inversion. So, two-fold rotation with one inversion.

Now, point to be noted is if it would have reflected, then also would have seen the same thing. So, if we put a plane here, if we put a plane here, maybe, and with respect to this, we can see that these two are mirror images of these two, which means we could have avoided the rotation and inversion just by doing the reflection also. So, it is equivalent to reflection. Now, here, the plane of rotation is the vertical axis, and the plane of reflection is the horizontal. The plane of reflection is horizontal, which means the plane of reflection is perpendicular to the axis of rotation.

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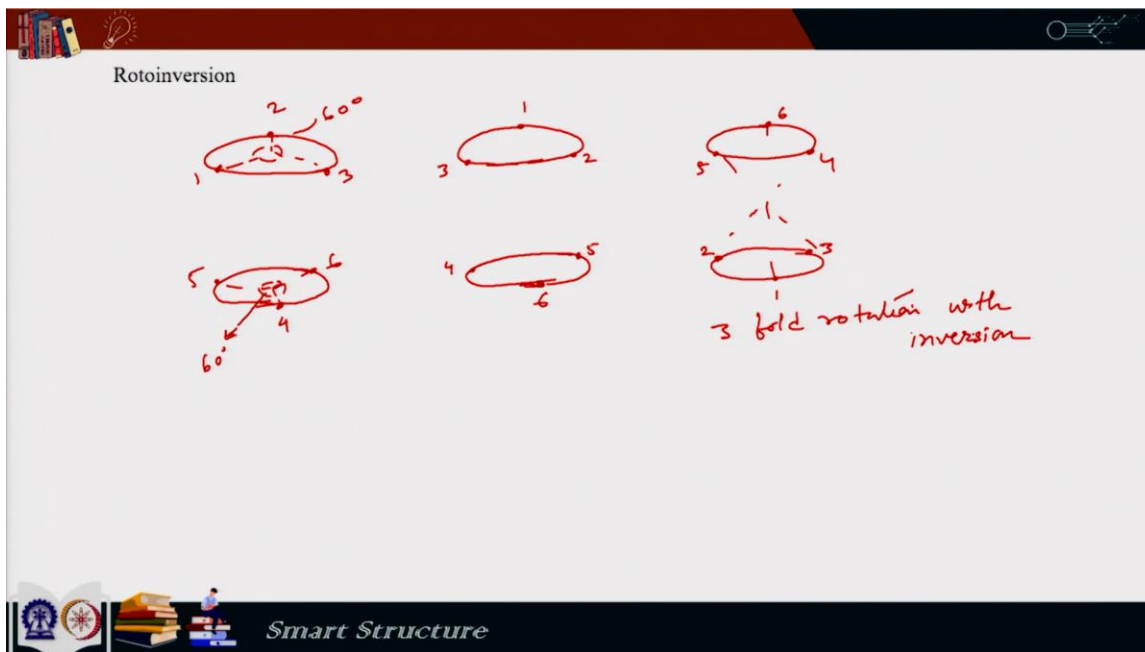


Now, we will talk about a three-fold rotoinversion. So, let us again imagine three points now; we will think of one, two, three, and then we have four, five, six. Now, to get this shape back, what needs to be done is they all need to be rotated by an angle 360 degrees. So, first of all, we can see that they all are oriented at an angle 60 degrees. So this, this, this, they all are 60 degrees and same here also, they all are oriented.

So, the angle between, so that these two successive points they make an angle of 60 degrees. Now, if we do a one-fold rotation, sorry, I mean, if we do a rotation by an angle 60 degrees, then what happens is our point, our point one comes here, point two comes here, and point three comes here, and then here what we see is point four comes here, point

five comes here, and point six comes here. Now, if they are rotated and if the places are interchanged, then so then, we will see that point one comes to this point, and then point two comes here, and point three comes here, and point six comes here, and point five comes here, and point four comes here. So the shape is back, so that is a three-fold rotation with inversion.

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Now, we will talk about a six-fold rotation with inversion. Okay, now, we will talk about a six-fold rotation with inversion. So let us imagine a situation like this. We have the atoms arranged in this fashion, and two successive atoms make an angle of 30 degrees at the center here. Again, we can see that if we rotate it by an angle 30 degrees, and then we invert it, then it becomes, I mean, we get the same shape. If we rotate it by an angle 30 degrees, so six-fold rotation plus inversion, we can see here, and also we can visualize it in other ways. So we can, instead of doing a three-fold rotation, if we do a six, sorry, instead of doing a six-fold rotation, if we do a three-fold rotation and then we reflect it, then also we get the same shape back. So, it is equivalent to a three-fold rotation and inversion. (Refer Slide Time: 25:28)

Rotoinversion

6 fold rotation
+ inversion
|||
3 fold rotation
inversion

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Based on the symmetries, various point groups can be defined for crystals. Here, we will talk about a point group in 2D. So, in two dimensions, there are ten point groups and these are denoted by the circles, dots, and lines. The first one is one. It is denoted by the circle with this one dot. Now, to get this configuration back, this circle needs to be rotated by an angle 360 degrees. So, it is a one-fold rotation. So that is why it is one.

Here, we can see this configuration again; to get this back, it needs to be rotated by an angle 180 degrees. So it is just two, and in both the cases, there are no reflections. So, I cannot define any line with respect to which the two parts can become mirror images of each other. That is why I do not have m here.

Here, we have both one and m. One because to get it back again, I need to rotate by 360 degrees. So it is one, and this line forms a, if I draw a line here, that forms a mirror because with respect to which, with respect to this line, the two parts become a mirror image of each other. So it is one m.

Here, we have two m m, two because if we give 180 degree rotation, the configuration comes back. So it is two, two-fold rotation, and there are two types of mirrors. If I draw a line here, that means if I put a mirror here, we get two mirror images, so this part is mirror image of this; this part is mirror image of this. Similarly, this line also divides it into two halves, which are mirror images of each other. So it is two m m.

Here, we have four because after 90 degree rotation, we get this configuration back, but there is no reflection symmetry here, so it is four.

This is four m m because after 90 degrees' rotation, the configuration comes back, and there are two types of mirrors. So if I draw a line here and if I draw a line here, there are same types of mirror because the mirror images that we get by this line is similar to the mirror images that we get by this line. But if we draw a line here, and if we draw a line here, that creates different types of mirror images. So although there are total four number of mirrors, the types are two, so it is four m m. So, it is not the number of mirrors; it is the mirror types that matter, so it is four m m.

Then comes three. If we rotate it by 120 degrees, the configuration comes back, but there is no mirror, so it is three. Here, if we rotate by 60 degrees, the configuration comes back, so it is six, there is no mirror.

This is three m because if we rotate it by 60 degrees, 120 degrees, the configuration comes back, so it is three, and here we have one with respect to this line we get mirror image with respect to this line, we get mirror image, with respect to this line, we get mirror image but all these mirrors are similar of same type, so it is three m.

Here, we have six because if we rotate it by 60 degrees, we get the configuration back, so it is six, and this line creates one type of mirror image, so there is mirror of one type, and if I draw a line here, or line through this or a line through this, that creates another type of mirror. So there are two types of mirrors, so it is six m m.

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Point Groups in 2D

1	2	1m (m)	2mm (mm)
4	4mm (mm)	3	
6	3m	6mm (6m)	

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Now, we will move to 3D, 3D crystals. So, there are generally seven types of 3D crystals. One is simple cubic. As the name says, it is a cube. So, a b c, all the lengths are same, and

all the angles are 90 degrees here. Tetragonal, it is a and b are same, but the vertical axis c is different, and all the angles are 90 degrees. Then comes orthorhombic. Here, all the sides are different a b c, they are not same, but all the angles are 90 degrees. Rhombohedral. All the axes, I mean, all the sides are same, but I mean, none of the angles are 90 degrees. And then comes monoclinic in monoclinic, none of the sides are same, two of the angles are 90 degrees, and the other one is not 90 degrees. Triclinic. None of the lengths are same, and none of the angles are 90 degrees. In hexagonal, we can see that a and b, they are same, but c is different, and there is one angle, which is 120 degrees. So these are all 3D different crystals.

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3D Crystal Types

Crystal Type	Axis Lengths	Angles
Simple 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	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$
Monoclinic	$a \neq b \neq c$	$\beta = \gamma, \alpha \neq 90^\circ$
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$

The unit cells of the seven types of crystal systems along with the relation among their unit cell parameters.

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Now, in the next class, we will look into the 3D point groups, and then from there, we will see how piezoelectricity comes into picture.

Thank you.