Acoustic Materials and Metamaterials

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Lecture – 35
Fundamental of Crystals

Welcome to lecture number 35 in the series on Acoustic Materials and Metamaterials. It is the last lecture of this week and we had began our discussion in the last class about sonic crystal. So, it was a lecture on Introduction to sonic crystals. So, in this class we will continue with our discussion on some of the Fundamentals related to Crystals. So, we have already studied some terminology as in what is meant by a crystal, what is meant by a lattice or a crystal lattice, then what are the two different types of arrangements possible etcetera.

So, in this class we will start with a discussion about what is meant by a real space and a Reciprocal space and then followed by that there will be related to a real space, we have a Real lattice or a direct lattice and related to the reciprocal space, we have a reciprocal lattice.

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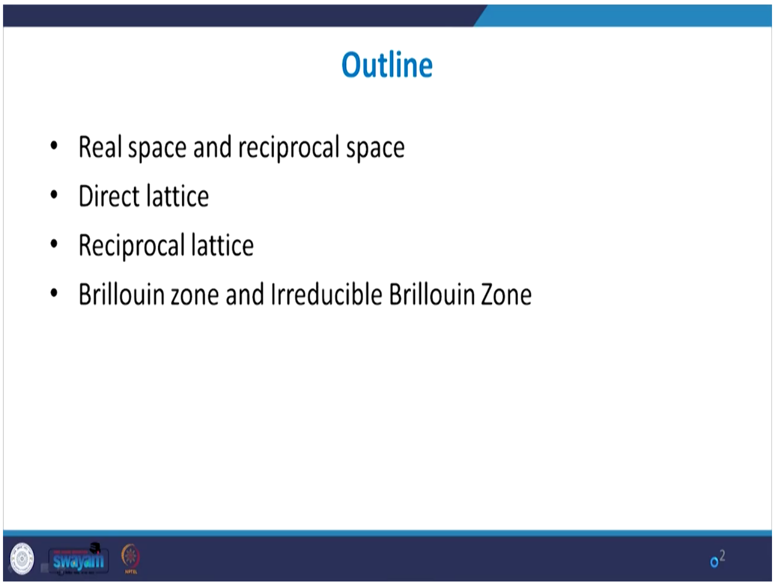

And then we will conclude our discussion with what is meant by a Brillouin zone and an Irreducible Brillouin zone and these two concepts are very important because from now on when we study about sonic crystals, so all the response that is studied for the sonic crystals will only be studied in the irreducible Brillouin zone.

So, that is the zone within which the response characteristics of all these crystals will be studied. So, what is meant by a real space? So, first of all a direct lattice. What is a direct lattice? It is a lattice in the physical lattice structure or the physical crystal lattice that we have been discussing. So far that is the direct lattice or whatever we can see in the real in the real space that crystal structure or crystal lattice is the direct lattice.

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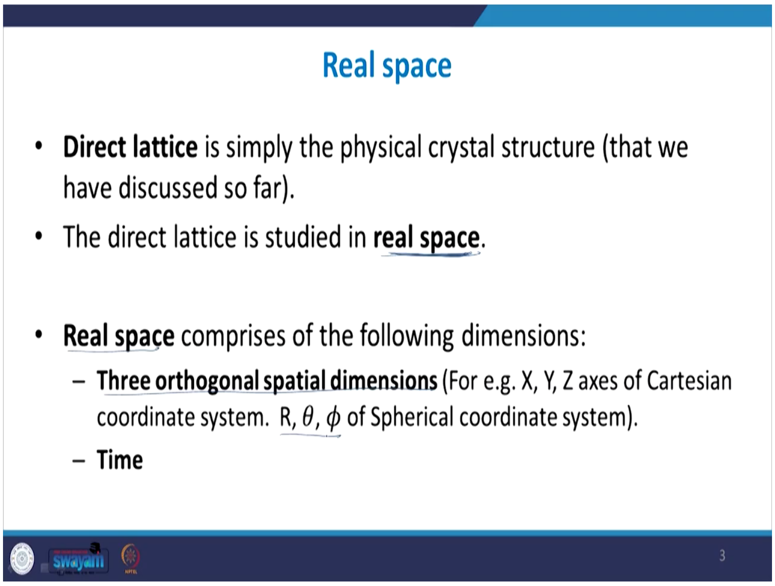

So, the direct lattice it is studied in the real space. So, what is meant by a real space? Now we know that we know that a typical space consists of the three spatial dimensions as well as a time dimension. So, a real space consists of three orthogonal spatial dimensions. So, if you are taking irrespective of what kind of system you are studying, so let us say you choose Cartesian coordinate system.

So, in that case you will have three independent special dimensions. It will be the X axis, the Y axis and the Z axis, they are all of three. They are mutually perpendicular to each other and mutually independent of each other. In the same way let us say you choose a spherical coordinate system.

In that case, any point can be represented the location of any point can be represented by three independent coordinates which is the R theta and phi. So, here R is simply the radial distance from the origin and theta is the angle that the reflection, it is the angle that the reflection of the point makes with the X axis and phi is the angle that the radial vector of the point makes with the XY plane. So, we have studied about what is a Spherical system or what is a Cartesian coordinate system.

So, whatever system we follow we for any for any object, the location can be fully described by the three spatial coordinates and by a fourth dimension which is the time. So, we have the space time coordinate and this constitutes a real space.

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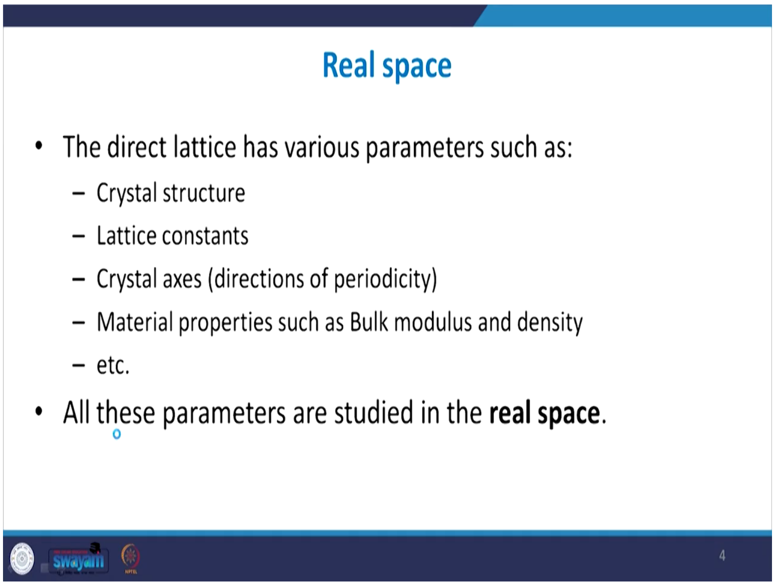

So, all the things that we have been studying for our crystal lattice such as what is the form of crystal, what is the shape size and the dimension of the crystal, what are the various directions of periodicity, the various lattice constants even the properties such as bulk modulus and density, all of this is has been studied in a Real space.

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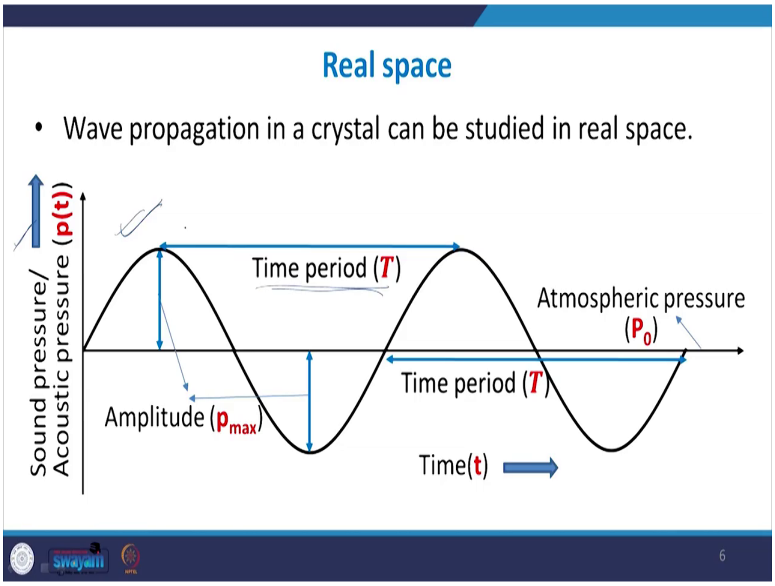

But we can also study Wave propagation in a real space. So, in the very beginning of this course in the lecture 1, I told you that any wave propagation specific specifically an Acoustic wave propagation can be described as a periodic variation in space and time.

So, if it is sum let us say if it is a standing wave, then that becomes a periodic variation over time, but over space it remains constant. In the same way we have, but the typical acoustic waves they are travelling waves because they are propagating and transferring the sound energy from the source to the receiver. So, they are the travelling waves and the typical traveling wave is then a disturbance which can be shown as a periodic variation of a space and time.

So, wave propagation can be represented in the real space like this. So, you have the variation of Acoustic pressure over space and an important parameter that you get is wavelength which is the distance over space or the spatial distance over which the wave is repeating its pattern. So, when you represent it and see what is how the wave is varying over this, over any one of the spatial dimension. So, when you have three spatial dimensions let us say X Y and Z and you get and you create a 3D wave, then it will have a wavelength associated with the X direction, a wavelength associated with the Y direction and a wavelength associated with the Z direction.

So, across all these individual spatial dimensions you get a specific parameter which is called as a Wavelength. Similarly the wave can be represented over the dimension time. So, it is like a periodic variation over time. So, if you see in this figure here and here the parameter that we get is a time period. So, here the wave is repeating its pattern over this time period. So, this is that length in the time axis or the distance along the time dimension over which the wave pattern repeats. Just the same way the distance over which the wave pattern repeats in the spatial dimension, we get a wave length and across a time dimension, we get a time period.

So, this is how the wave is in the real space, but we also studied that the just knowing the knowledge of how it is varying over space and time is not sufficient enough. In fact, what frequency components does it comprise of and how does the magnitude or the power vary over frequency or what you in general call as the power frequency spectrum is even more important because most of the noise control applications, they it means that they use the human ear and the human ear is highly frequency selective. Therefore, a knowledge of the frequency component becomes very important. Therefore, if any sound signal is available to you, so let us say in any noise control application you acquire some sound signal and that sound signal will be the sound signal in the real space.

So, it will be a sound signal varying over space and time, the spatial dimension and time, but you convert that sound signal into a new domain which is the frequency and wave number domain. So, you do a Fourier transform. So, if you want to study the wave propagation in even more detail, then just acquiring a signal is not sufficient. You sometimes have to study it in a different framework by using Fourier transform, so that you can get a more detailed information of what are the individual frequency components and what are the various wave numbers or wave propagation vectors. So, this creates the need for using a reciprocal space.

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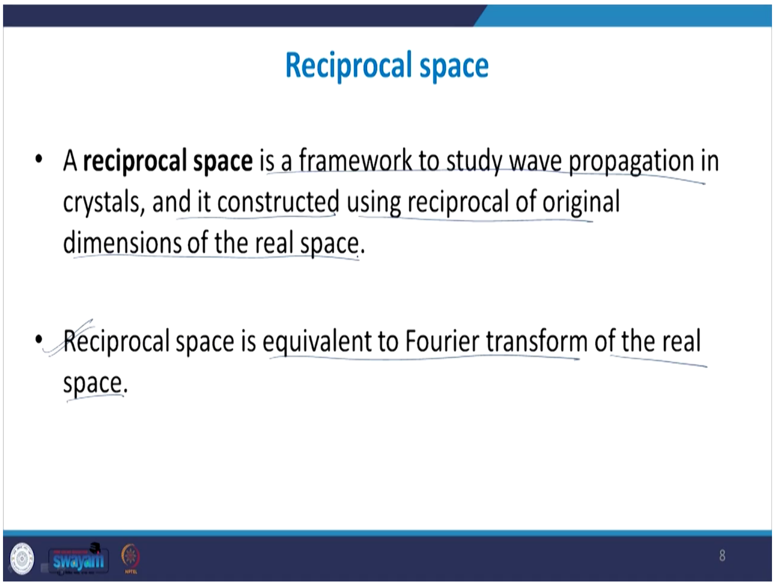

So, within the crystals also let us say we are studying the wave propagation in the crystal, then we can either study the wave propagation in the normal real space which is the spatial dimension in the time, but we can also create a reciprocal space. So, what we have is that we have a crystal it can be represented in a new framework altogether and that new framework will show you the relationship of how the wave is propagating over the different frequencies and over the different sort of wave numbers.

So, reciprocal space can be thought of as it is equivalent to doing a Fourier transform of the real space. So, to get a more detailed analysis of wave propagation, we can study it by doing a Fourier transform of the real space. So, this is a framework that is used to study wave propagation and it is constructed using the reciprocal of the original dimensions of the real space.

So, as a name suggests it is reciprocal space which means that whatever was the real space, we use reciprocal of the dimensions. So, we reciprocate the quantities to get a new sort of framework where we study the wave propagation and this new framework will give you more detailed information about the frequency components of the wave.

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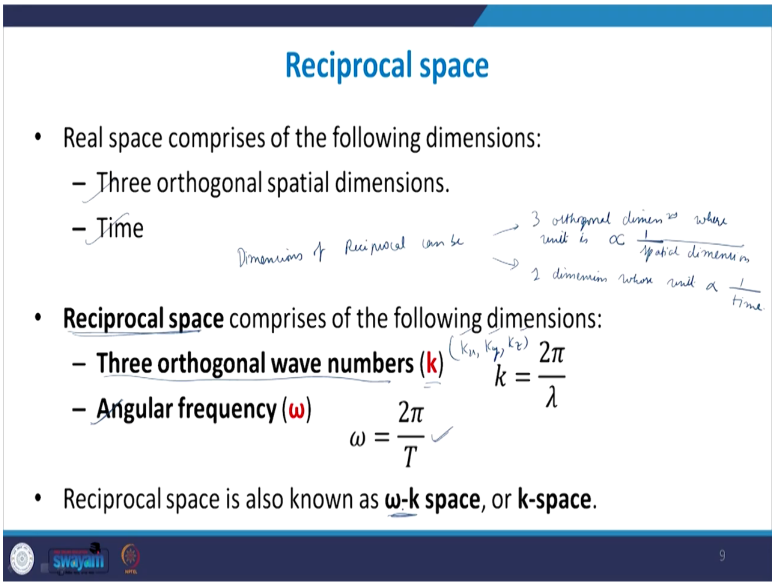

So, now we know that the real space it comprises of three orthogonal spatial dimensions X Y Z and the time axis. So, if you have to think of a reciprocal space, so for a reciprocal space you will need some reverse of the spatial dimension and some reciprocal of the time dimension to something. So, the dimensions for reciprocal space, so here the dimensions of a reciprocal space can be three orthogonal dimensions where the unit is proportional to 1 by the spatial dimension, 1 by the spatial dimension in the same way.

So, these and it can comprise of one dimension whose unit is the directly proportional to the reciprocal of the time. So, we are using the reciprocal of the quantities that is used in the real space to get a new framework. Now, we know of two important parameters that was wave length and time period in the real space. So, if we reciprocate the wave length which is 1 by lambda and then add 2 pi to it.

So, 2 pi by lambda as you know is a very important number which is the wave number or the propagation vector. Similarly you can do 2 pi by capital T which gives you the angular frequency which is again omega, a very important parameter for a wave. So, an optimum choice could be that we create a reciprocal space using omega and k as the dimensions. So, what you get here is that. So, the typical reciprocal space is created using the three orthogonal wave number dimensions.

So, with every so there is let us say we had x y and z axis, then corresponding to every direction we have an individual wave propagation vector. So, there we have a wave propagation vector along the x direction, a wave propagation vector along the y direction and a wave propagation vector along the z direction. So, you have kx, ky and kz. These are the three independent components of the total k vector.

So, these are kx, ky and kz; k, ky and kz. So, these are the three individual wave vectors or wave numbers and they represent the three orthogonal wave number dimensions. So, these are three first three dimensions are kx, ky and kz and the fourth dimension is then 2 pi by capital T which is the angular frequency dimension

So, when this form of framework is used where you have k space, where you have a reciprocal space which comprises of the omega k space. So, you have instead of having the spatial location and time, now you are using what is the frequency and the wave number and you are representing the various waves in terms of these coordinates, then that becomes a reciprocal space which is also called as omega k space or simply the k space.

So, now you know why do we use reciprocal space, it is to get more detailed analysis of the frequency components and the propagation of the wave. So, the same lattice which we studied in the direct in the real space can then be converted into a reciprocal space.

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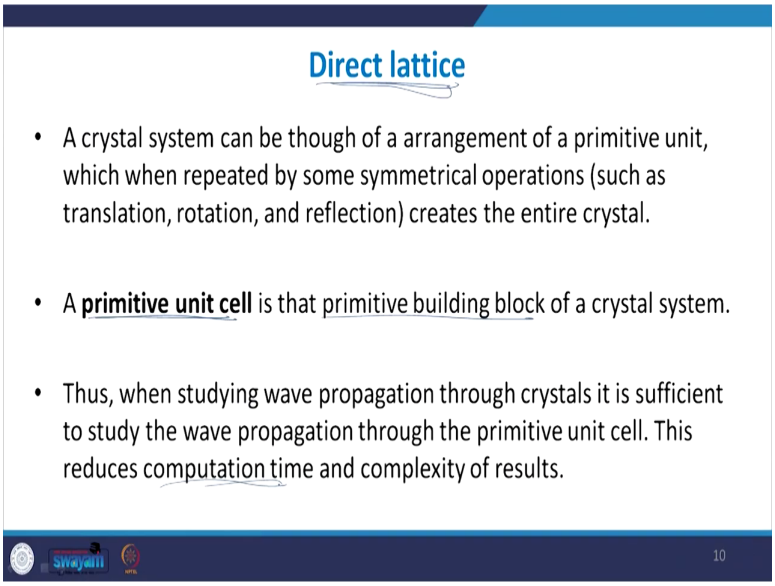

So, let us study direct lattice which we know is the lattice represented in the real space. Now every lattice can be thought of as some repetition of a primary building block.

So, you and that same building block when it is repeated using some symmetrical operations like if it is translated or it is rotated or it is reflected about some axis, it can create the entire crystal, so that you primitive unit becomes the primitive unit cell or simply the primitive building block of the crystal system.

Now, if we know; if we know how the wave propagation occurs in this particular primitive cell and we know that that is because a lattice is actually a periodic arrangement, it is a very strong ordered periodic arrangement. So, if we can find out what is the minimum zone or the minimum the main a smallest repeating unit which on repeating is creating the entire crystal, then in then we can study.

So, instead of studying the wave propagation over the entire domain of the crystal, we can just study the wave propagation over this repeating unit and we can reflect or we can simply we can simply translate or reflect the results over the other over we can keep reflecting it, so that we get the results over the entire crystal so just to reduce the computation time in how to calculate.

So, sometimes you use MATLAB or sometimes you use some finite element methods to compute or many other numerical tools to compute how the wave should propagate within different crystals. So, you can reduce the computation time if you reduce the computational zone. So, instead of now studying for the entire crystal, you can just study within a small repeating unit and then you know that the result that we are getting for this repeating unit it will be symmetrical because the crystal is symmetrical, the repeating unit can be symmetrically many such symmetrical units can be arranged to get the entire crystal.

So, the result will be the same for the crystal. So, whatever result you get within a primary unit, it can be then used to create the solution for the entire crystal. So, to reduce computation time sometimes only wave propagation is studied within the primary unit cell.

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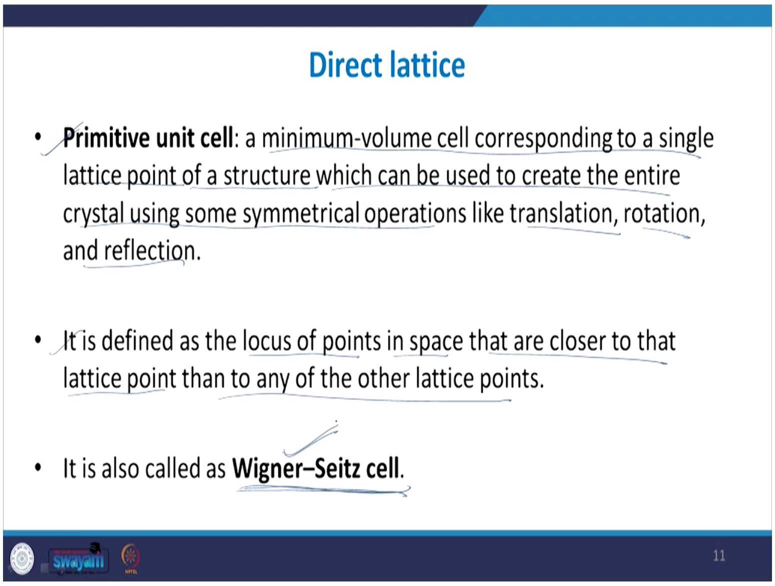

So, what is the definition? The formal definition of this primitive unit cell, it is the minimum volume cell which corresponds to a single lattice point of a structure which can be used to create the entire crystal using some symmetrical operations like translation, rotation and reflection.

So, it is the minimum volume of the cell with just one lattice point which can act as the repeating unit to create the entire crystal and another way of defining it can be the locus of points in a space that are closer to that lattice point.

So, suppose we have a crystal, we choose one point and we want to and we want to create a primitive unit cell around that one lattice point, then it will be the locus of all the points which are closer to that particular lattice point than to any other lattice points and since this kind this kind of particular cell that we create is called as the Wigner-Seitz cell. So, it is named after the scientists who discovered it and proposed this idea of Wigner and Seitz. So, the primitive unit cell sometimes is also called as the Wigner-Seitz cell.

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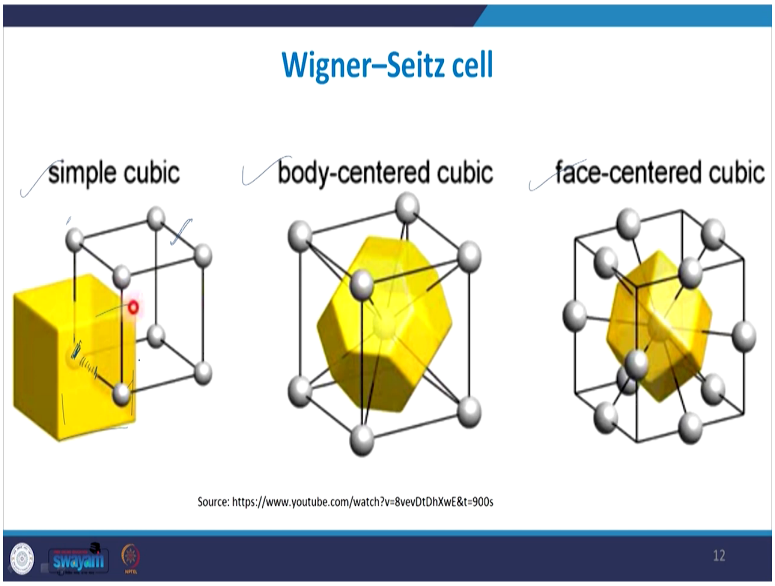

So, this shows this diagram here shows what are the different primitive units. So, let us say you have a cubic arrangement, then you have a cubic lattice, then a cubic lattice could be first broken down into its bravai lattice. So, the cubic lattice will give you a cubic structure.

So, this is the unit cell of the cubic lattice and within this unit cell also we can break it down to get what is the repeating unit which contains only in one lattice point. So, let us say we have chosen this as the lattice point, then we have to find out the volume of space or the entire locus of points which are more closer to this lattice point than to any other point. So, if you see the plane here, this is play, this is halfway through in this particular direction.

So, here any points within this zone, they will be more closer to this particular atom than to the other adjacent atom on the top. In the same way if you see the space this one this space here, it is also halfway. This plane is halfway into this sites side length. So, any so all the points which are within this particular between this point lattice point and the plane.

So, all these points here which are within the lattice point and the plane, they will be more closer to this lattice point compared to this adjacent lattice point and in the same way you can keep constructing such planes and you finally find a volume of space which is a cube itself and it passes through, it passes midway between all these lines. So, it is half way. So, the lines these are the connecting lines of the lattice points adjacent lattice points. So, halfway between that you have planes and within that you can get a cube.

So, this shows us the primitive repeating unit for a cubic structure. In the same way you can get some Wigner-Seitz cell or a primitive repeating cell or the primitive primary what we call it as a primitive unit cell, this comes out to be this. So, always what you do is you choose a particular lattice point and see what could be the volume of space which is which contains the points which are closest to this and not to any other lattice point and then you create a volume of space that becomes the primary repeating unit which on repetition can create the entire lattice structure. Just like we have the primitive unit cell, we also have another parameter which is called as a primitive lattice vector.

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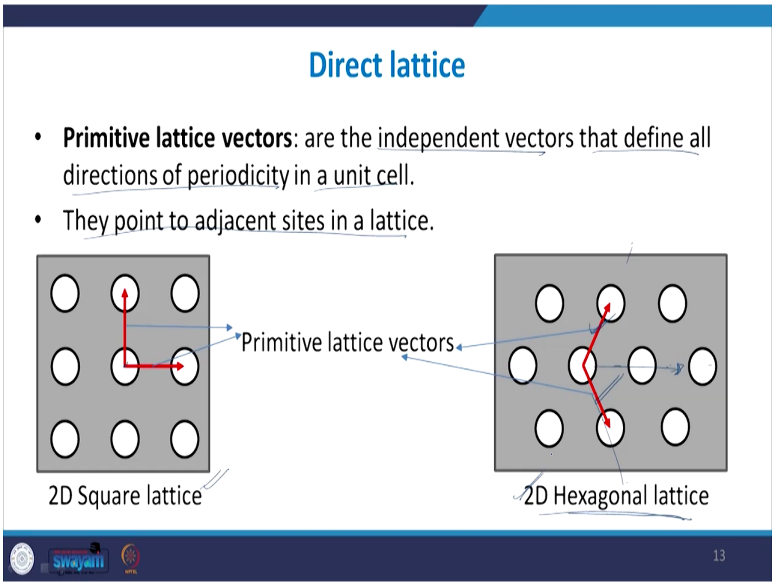

So, these are those independent vectors that define all directions of periodicity in a unit cell. So, let us say and the point to the adjacent sites in the lattice, so let us say we have some. So, it is better to show it in the two dimension for a better visualization. So, let us say we have 2D square lattice system.

So, these two; these two vectors will become the primitive lattice vectors because you can see there is a periodicity along the horizontal direction and a periodicity along the vertical direction. So, we can choose one point as the lattice point or the primitive lattice point and then, we have the vectors which join the center of this origin to this to the center of the next adjacent lattice point.

So, this is the length which the length will be same as the distance between the centers of two adjacent lattice points or lattice pairs. So, this is what you get and they correspond to the individual directions where periodic variation is happening in the same way you can for a hexagonal lattice. You get these as the primitive lattice vectors and you can say that any other repetition.

So, there is a repetition happening in this direction, there is a repetition happening in this direction and there is also a repetition in this direction this one, but this can be represented as a combination of the first two direction. So, this is not independent. So, we only have two independent directions here. So, these are the lattice vectors which is simply the direction over which periodic variation is happening and they are independent.

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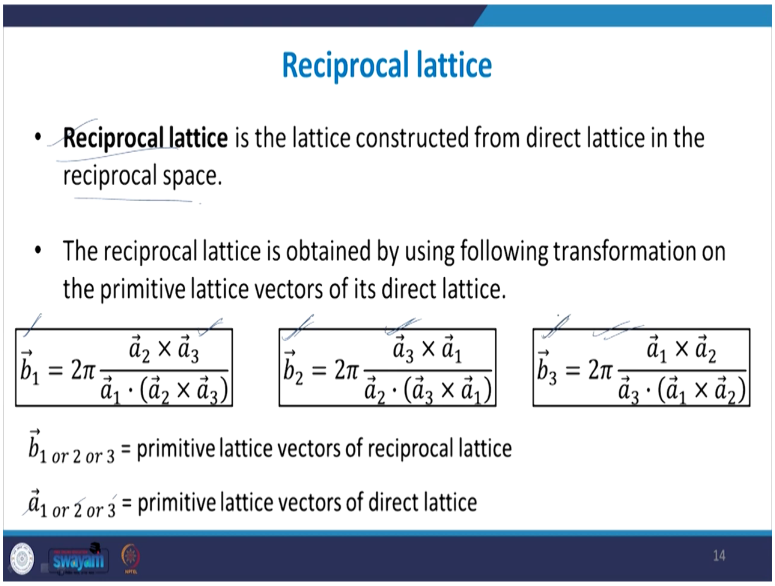

So, this is sort of a coordinate system for a direct lattice. Now, let us come to reciprocal lattice and study the same terms in the reciprocal lattice. So, what is a reciprocal lattice? It is simply the lattice which is constructed in the reciprocal space and how do we construct a reciprocal lattice.

So, let us say we have a 1 a 2 and a 3 as the primitive lattice vectors of a direct lattice. So, in the previous case we had a 2D system. So, we had only two lattice vectors, but if we have a 3D lattice system, then we will have three such lattice vectors a 1, a 2 and a 3 and if we do these transformation operations, then we will get the primitive lattice vectors for the reciprocal lattice and then based on that you can create the reciprocal lattice.

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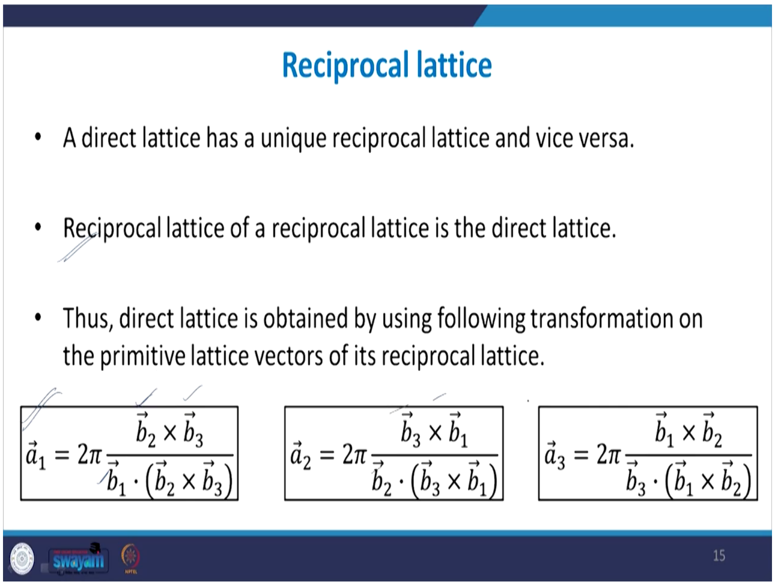

And this action is obviously it is it happens both ways. So, what do you mean by this is that for every direct lattice there will be a reciprocal lattice that will be unique so and the vice versa. In the same way just like let us say the example of Fourier transform I am going to give again. So, let us say you had a real signal in x and t for x y z and t.

So, it was a function of p as a function of x y z and t you did a Fourier transform and you got signal in the reciprocal space. So, you got some p as a function of omega and k, you again do a Fourier transform. So, what you will get is that you will again get the actual signal back which will be p as a function of xyz and t.

So, what you do is that if you do this operation twice, you get the real signal back. In the same way let us say you create a reciprocal lattice of a reciprocal lattice, then you will get the direct lattice. So, if the same transformation is again done to the reciprocal lattice vectors, you get the direct lattice vectors.

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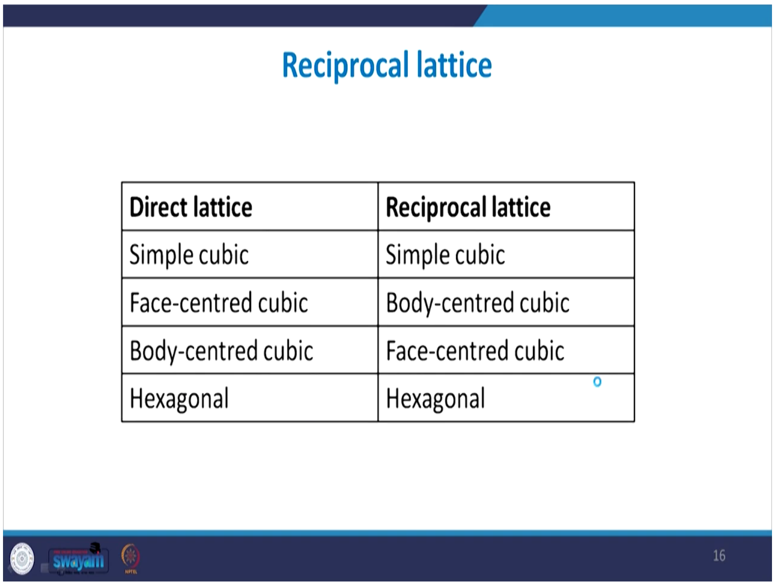

Reciprocal lattice

Direct lattice	Reciprocal lattice
Simple cubic	Simple cubic
Face-centred cubic	Body-centred cubic
Body-centred cubic	Face-centred cubic
Hexagonal	Hexagonal

So, it has been found in these studies of crystals is that a simple cubic generates a simple cubic reciprocal lattice, face-centered generates body centered, body-centered face-centered and hexagonal generates another hexagonal lattice as the reciprocal lattice.

So, the shape for hexagonal and simple cubic remains the same. The dimensions will obviously change which will be governed by these transformation equations, but the shape will be the same.

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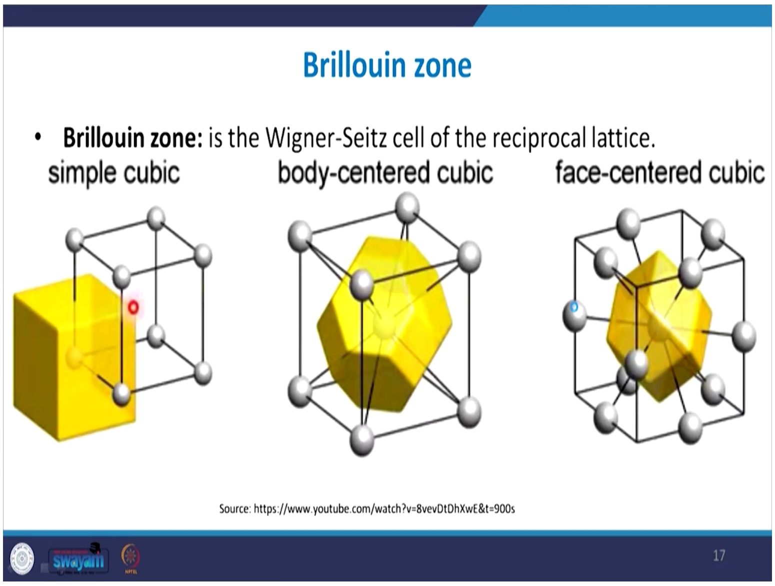

Now, the last concept in this particular lecture is brillouin zone. So, just like we had a primitive unit cell or a Wigner-Seitz cell for a direct lattice, so now we have a reciprocal lattice. If you find out what is the Wigner-Seitz cell for this reciprocal lattice, that will be your brillouin zone.

So, first you have a crystal, you convert it into its reciprocal lattice and then you find out what is the minimum repeating unit with just one lattice point. So, that will give you the brillouin zone. So, what we can do is that let us say we want to study the wave propagation in a crystal. We can reduce the crystal into its brillouin zone just to reduce the computation time and we can study the wave propagation only within the brillouin zone and based on the knowledge we get that can be for transfer to create the in to get the knowledge of what is happening in the entire crystal.

So, just by studying a small zone we can get the knowledge of what is happening in the entire crystal. However if you see these brillouin zones here, they are also have symmetry. So, the brilouin zone itself can be reduced even further and further down ah, so that we get the smallest zone which we can study and recreate the result for the entire crystal.

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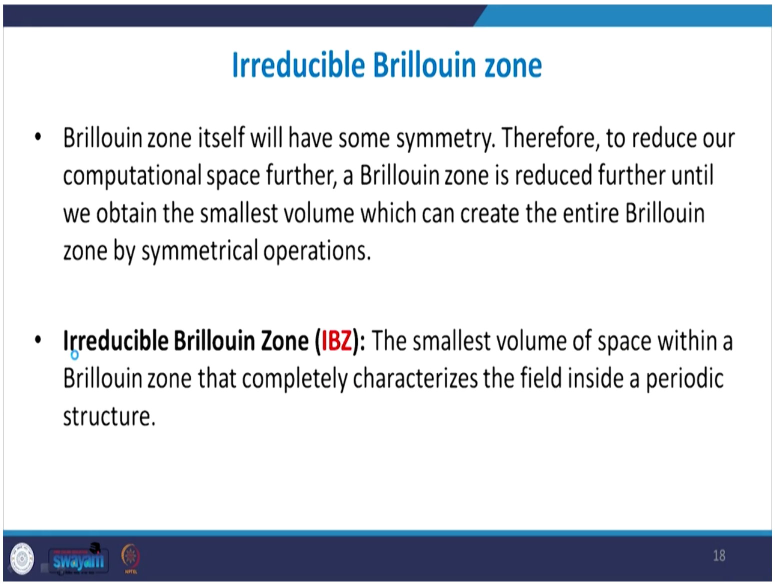

So, that gives the concept of Irreducible Brillouin zone. So, the Brillouin zone that we are obtaining can also be symmetrical in nature. So, we can cut down the zones into the various portions of symmetry and get the smallest unit which on repetition will create the Brillouin zone and this Brillouin zone on the repetition will create the entire crystal.

So, IBZ is a very important concept because from now on when we study about the response of sonic crystals, we will always see the response in the in the one of the axis will be the IBZ or the Irreducible Brillouin Zone because the how the wave propagate will only be studied in the Irreducible Brillouin zone of the sonic crystal and that can give you the idea of what will be happening in the entire crystal Brillouin. So, this is just to reduce the computation time and save safe computation time and the complexity of the results.

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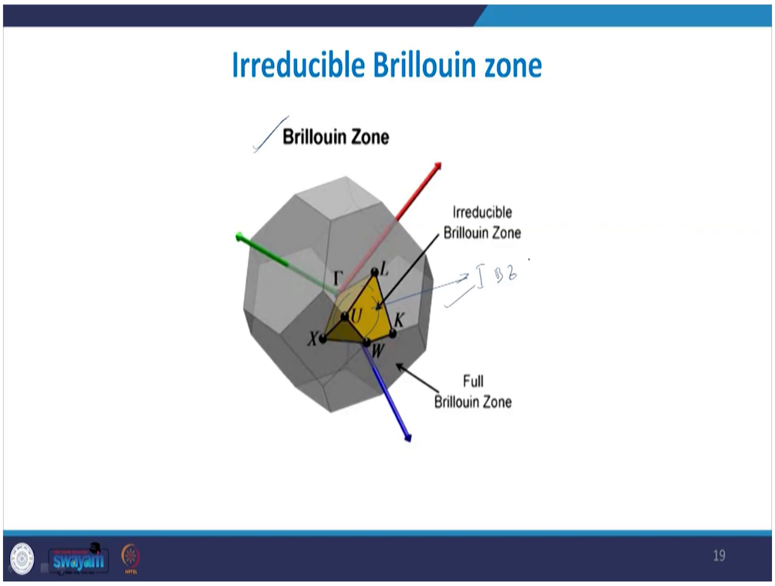

So, let us say if this is a particular crystal, this will this is the very small zone which is symmetrical and which on repetition is creating the Brillouin zone; so this is the IBZ. So, we will continue this discussion about irreducible Brillouin zone, then we will continue forward to discuss about band gaps in the next lecture.

So, thank you for listening.