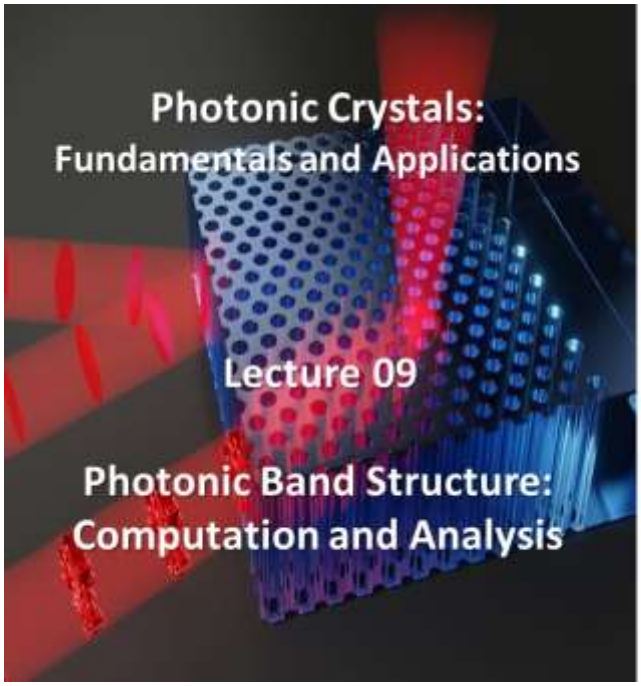


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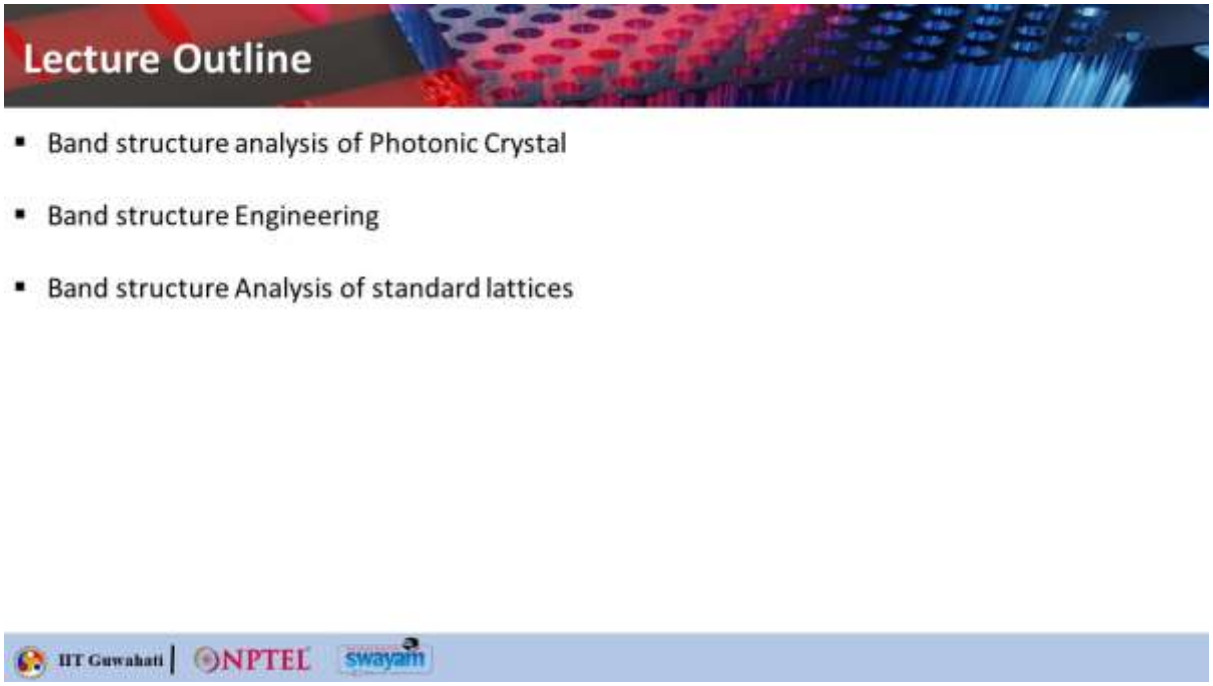
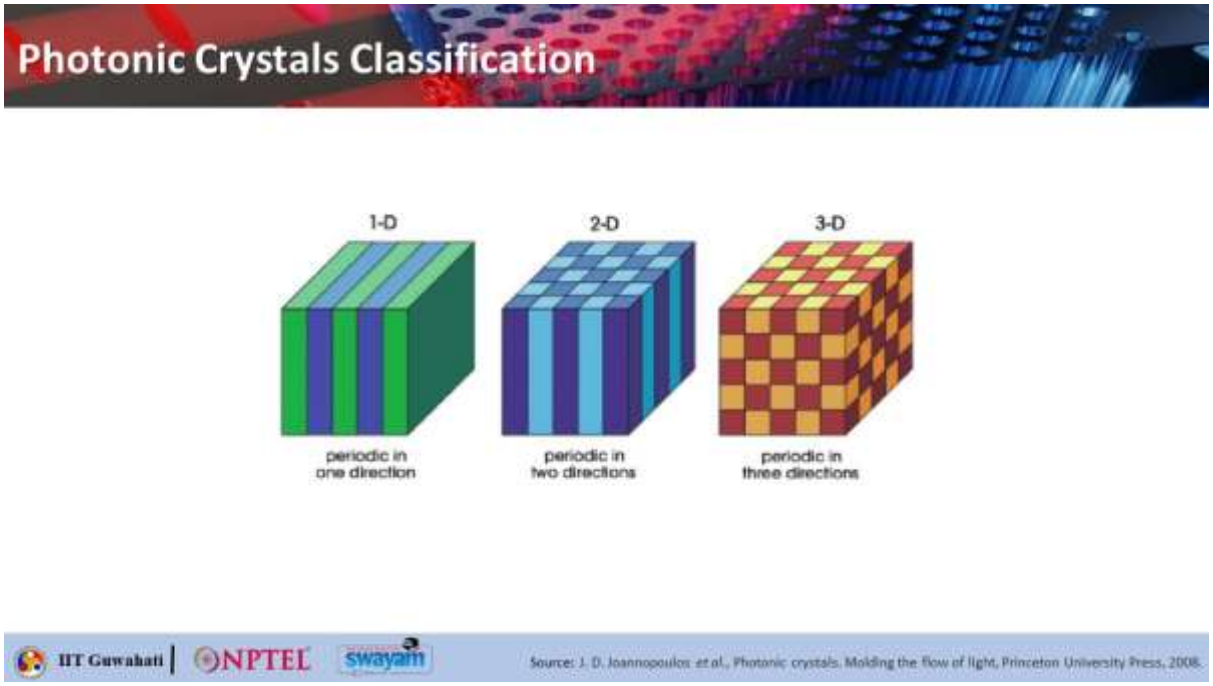
Lec 9: Photonic band Structure: Computation and Analysis

hello students welcome to lecture 9 of the online course on photonic crystals fundamentals and applications today's lecture will be on photonic band structure computation and analysis

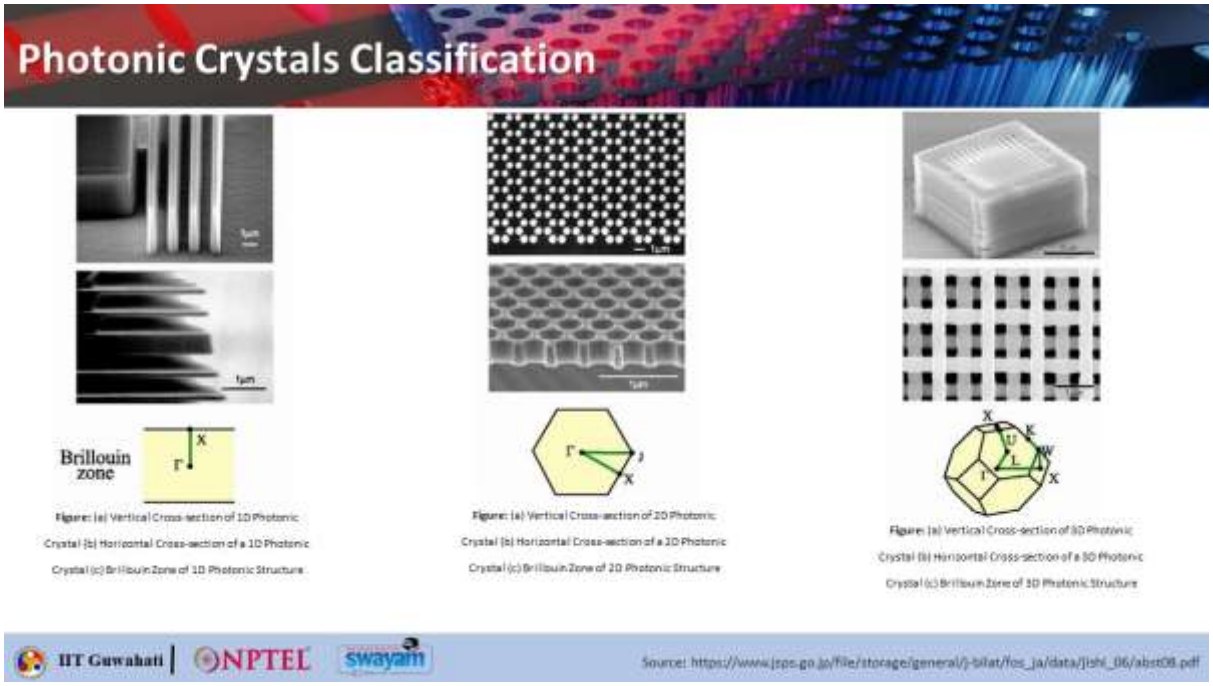



so here is the lecture outline today we shall be discussing band structure analysis of photonic crystal band structure  engineering and also analysis of band structure for the standard lattices

# Band structure analysis of Photonic Crystal




so, let's start with this particular topic So, here you can see the image of 1D, 2D and 3D photonic crystals ok. So, these are basically periodic arrangement of dielectric objects right. And one important thing to remember here is that lattice constant is basically comparable to the wavelength of light. Now, this photonic crystal is new artificially created materials in which refractive index is basically modulated periodically. And that scale or you can say the lattice constant is of the order of the wavelength of light of operation.



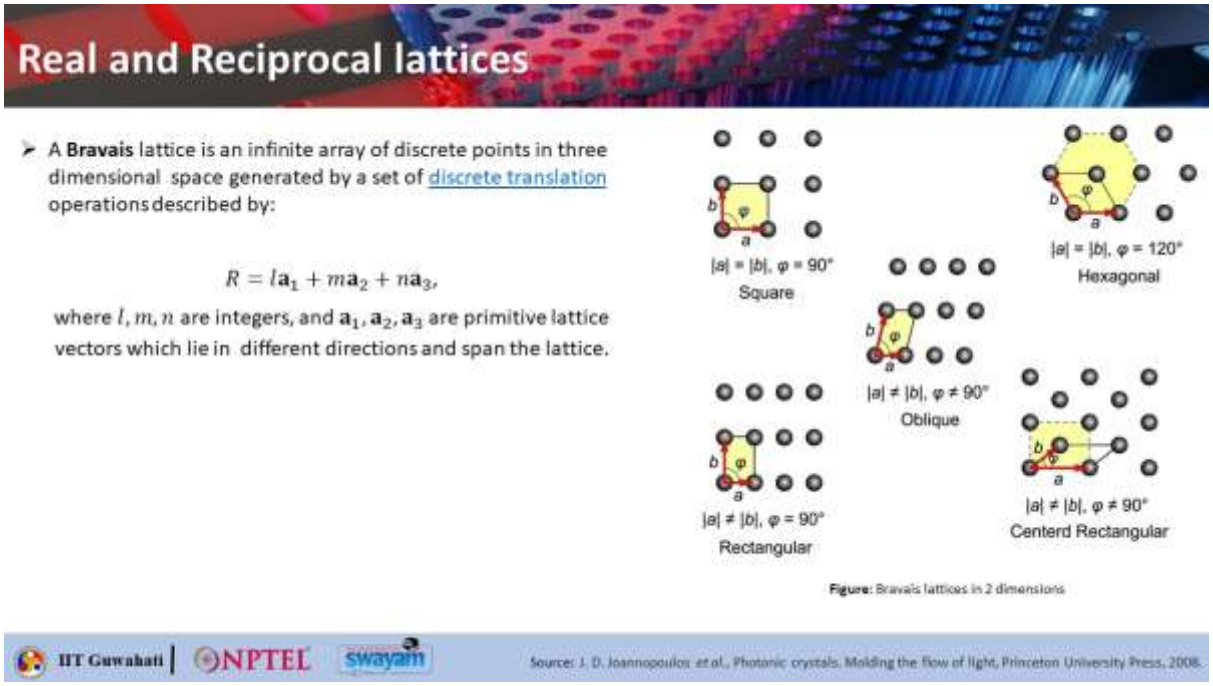

So here you can see three different photonic crystals.

So this is the vertical cross-section of the 1D photonic crystal. And this is a horizontal cross section of the same. So you have some material and then air, material, air, and so on. And this is the brilliance zone of the 1D photonic structure.

So the center is marked as gamma and middle of this particular edge is marked as X. So these are the two important points as you can see in this 1D photonic crystal. Here you can see a vertical cross section of 2D photonic crystal. It looks like a beautiful structure which is repeating periodically in both X and Y dimension. And this is the horizontal cross section.

So this tells you about you know, the height of the, you know, finite height of this particular crystal. And you can see these beautiful patterns which are seen here, right? So they are forming a nice hexagonal array, okay? So this is the Brillouin zone of this 2D photonic structure, which is also hexagonal in shape. So there are three important points here, which is gamma, J and X. okay and here is the vertical cross section of a 3d photonic crystal and this is the corresponding horizontal cross section and you can see this is the brilliant zone of this 3d photonic crystal and these are the important points which are marked here okay that tells you about the irreducible brilliant zone so we'll get to know the concept of brilliant zone in more details in this particular lecture and we will see that how these are calculated. Now why it is important because all these things enables us to engineer, create and engineer the photonic band gap and also allows us to localize light.

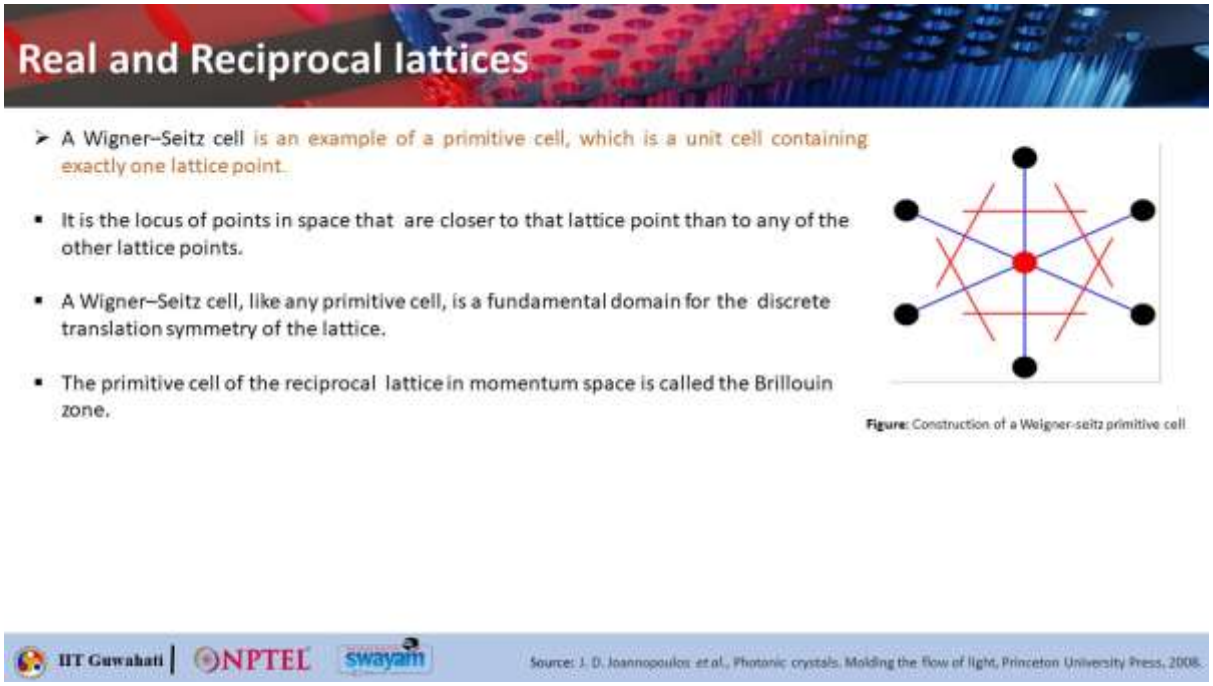
okay at a particular defect point. So these have potential in applications such as optics, optoelectronics, microwave techniques, quantum engineering, biophotonics, acoustics and so on. So there are lots of applications which we have already discussed before in the earlier lectures, initial lectures. But these are the photonic crystals that allow us to achieve those applications.




Now let us start with real and reciprocal lattice.

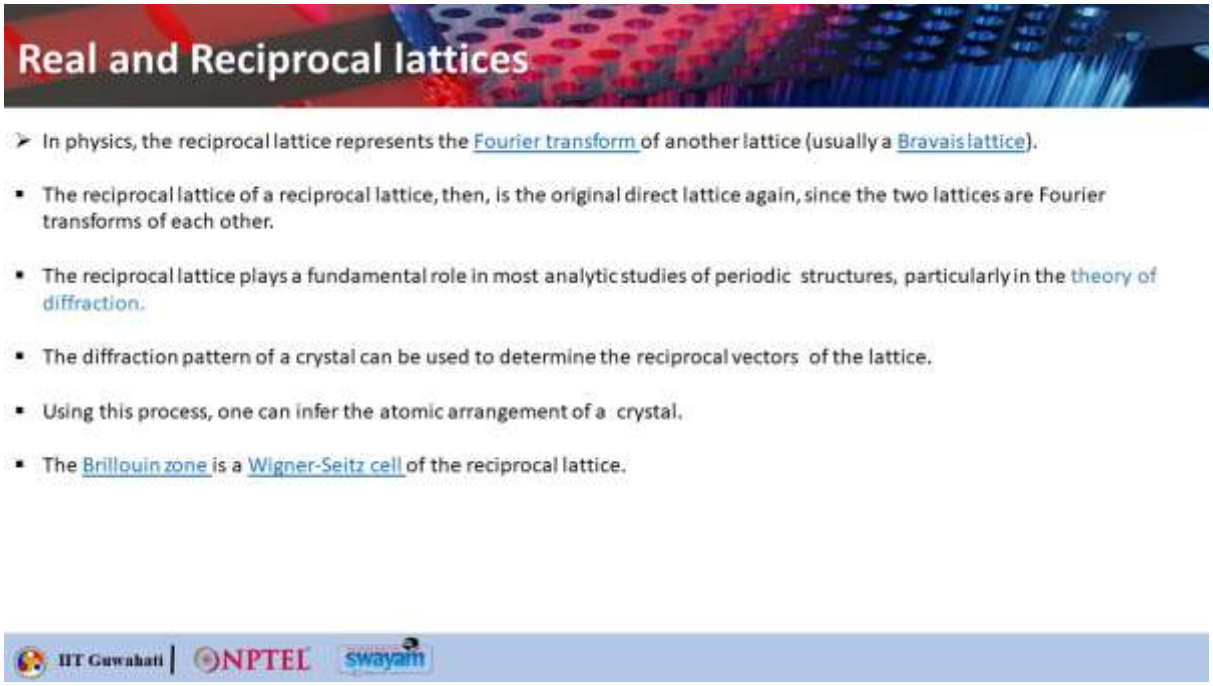
So this is how Bravais lattice or real lattice looks like. So, a Bravais lattice is basically an infinite array of discrete points as you can see. They can be in three-dimensional space depending on the periodicity of the crystal. So, for a 3-dimensional system you can write as L a1 plus m a2 plus n a3. So, a1 a2 and a3 are basically the primitive lattice vectors and L m and n are the integers right and this actually can form or you can refer to any, you know, translation along the lattice using this translational operation, okay, R.

And here is an example of Bravais lattice in two dimensions. Why we use two dimension and example? Because it is easy to visualize. Here we can see square, hexagonal, rectangular, oblique and centered rectangular. I am not going to details of these parameters which I have already discussed in the previous lecture or so. So, from that, what is important is that the concept of Wigner-Seitz cell.



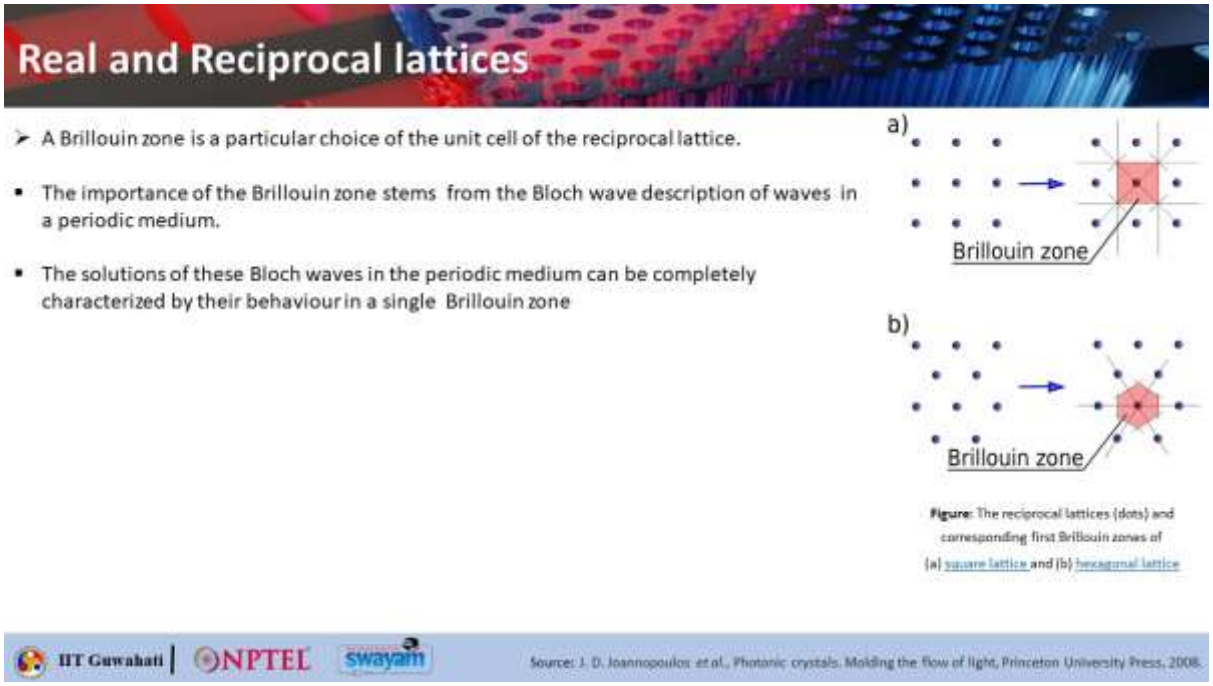

So how do you actually construct Wigner-Seitz primitive cell? So this is an example of a primitive cell in which a unit cell containing exactly one lattice point. So how do you do that? So you see this is the lattice. so you can only pick any particular lattice point and you can highlight it as red one okay and you want to find a region or locus of the points in space which are closer to this lattice point than any other lattice point. So, if you remember briefly how we discussed it in the previous lecture, you got to draw the lines connecting the neighboring lattice points and you got to draw the now perpendicular bisector. So, anything that within this region in this region will be closer to this atom or this lattice point than this lattice point right similarly if you take this connecting line and bisect it so the points within this region will be closer to this lattice point than this one and you repeat it for all so when you add up all the space you get this hexagonal region or space which is your wigner sheet cell So what is this Wigner says cell like any primitive cell is basically a fundamental domain for the discrete translational symmetry of the lattice.

So if you take this okay as a primitive cell and repeat it periodically you will be able to form the entire lattice. okay. And if you take the Fourier transform of this Wegener-Seitz cell, what will happen? You actually go to the reciprocal lattice space and the primitive cell in reciprocal lattice in the momentum space or the case space is called the Brillouin zone. right. So, it is very similar concept.




So, in physics the reciprocal lattice represents the Fourier transform of another lattice usually a Bravais lattice. So, Bravais lattice is the real lattice if you take Fourier transform you actually transform from x y coordinate space to momentum space which you can write as kx ky something like that ok. so the reciprocal lattice of a reciprocal lattice will give you back the original lattice right so it is something like you know because the two four the two lattices are fourier transform of each other so in normal usage the first lattice okay whose transform is represented by reciprocal lattice is usually a periodic special function in real space and is also known as the direct lattice So while the direct lattice exists in real space and is what one should commonly understand as a physical lattice, the reciprocal lattice actually exists in reciprocal space which is also known as the momentum space or K space. So, the reciprocal lattice is important because it plays a fundamental role in most analytical studies of periodic structures particularly in the you know theory of diffraction. So, the diffraction pattern of a crystal can be used to determine the reciprocal lattice vectors of the lattice.

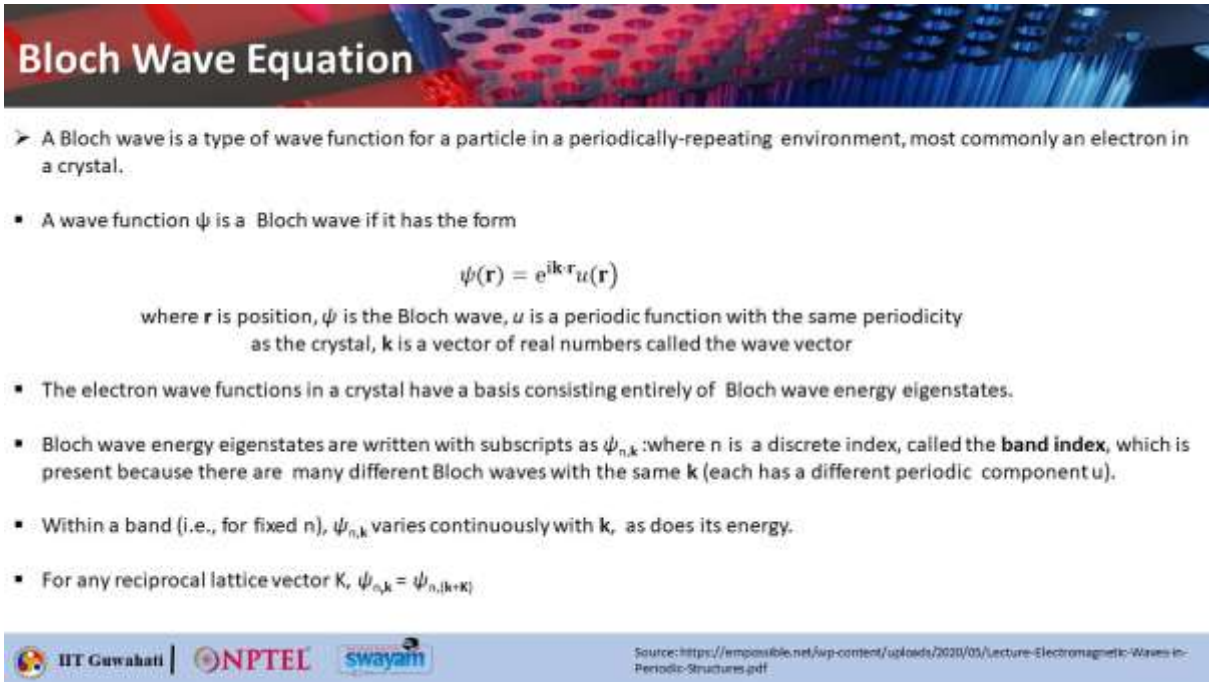
So using this process, one can infer the atomic arrangement of the lattice. It means if you take a lattice and record its diffraction pattern by shining light on it. So that diffraction pattern actually reveal the information of the reciprocal lattice and from that you can actually infer how the real lattice should look like.




So, a Brillouin zone is nothing but Wigner state cell of the reciprocal lattice. So, a Brillouin zone is basically a particular choice of the unit cell in the reciprocal lattice.

So, if you take a square lattice and you can actually, so this is basically a reciprocal lattice. okay and if you try to find out the brilliance zone using the same method that you only focus on this particular lattice point and try to draw the region which is closer to this adjacent points like this so you actually get this square Similarly, you can repeat the exercise for this hexagonal lattice or triangular lattice, and you end up getting a hexagonal pattern or hexagonal space as your Brillouin zone. Now, the importance of Brillouin zone stems from the block description of the waves in a periodic medium. In mathematics and solid state physics, the first Brillouin zone is uniquely defined primitive cell in reciprocal lattice. So, in the same way the Bravais lattice is divided into Wigner stage cell in the real lattice space, the reciprocal lattice is basically broken up into Brillouin zone.

And the boundaries of this cell are given by planes related to the points on the right. reciprocal lattice right. So the solutions of this block waves in the periodic medium can be completely characterized by their behavior in the in a single Brillouin zone. So Brillouin zone basically contains the information of how wave will propagate in the entire lattice. So if you only study the Brillouin zone you get to know about the entire lattice property.

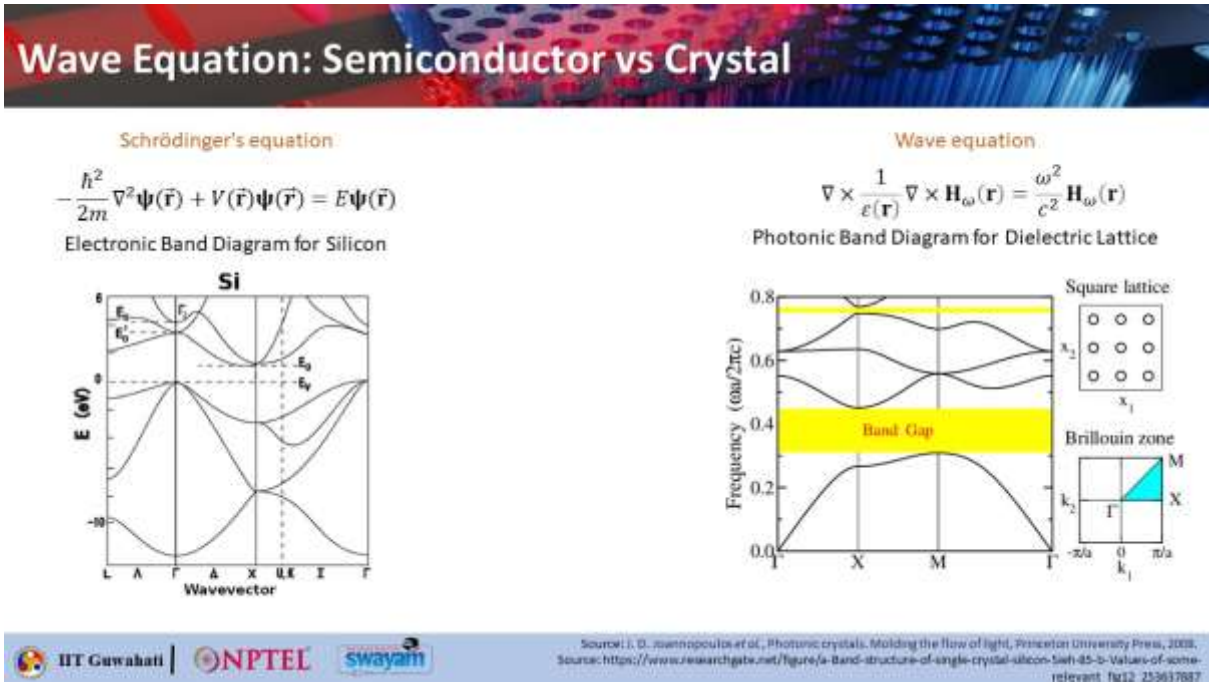



So now let us have a quick look on the block wave equation. So a block wave is a type of wave function for a particle in a periodically repeating environment. More commonly you can say something like an electron in a crystal. So if you consider a wave function psi is a block wave if it has got this particular form. So, if you can write $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$, where r is the position, $\psi$ is the block wave, u is basically a periodic function with the same periodicity as the crystal.

okay, then you can say that psi r is basically a block wave okay. So, what is k? k is the vector okay which is the wave vector right. Now, the electron wave functions in a crystal have a basis consisting entirely of the block wave energy eigenstates okay. So, this fact underlies the concept of electronic band structure.

right. So, block wave energy states are written with subscript psi and k where n will tell you about the band, okay. So, you can also say that n is the band index, right. So, it tells you that which band is present, okay because there are many different block waves with the same wave factor, okay. So, each may have different periodic exponent u. So, within a band that is for a fixed value of n ok psi n k varies continuously with k as does its energy of the band.

So, if you think of any reciprocal lattice vector k ok capital K. So, you can write $\psi_{n,\mathbf{k}}$ will be equal to $\psi_{n,(\mathbf{k}+K)}$. okay. That means all distinct block waves occur for k values within the first Brillouin zone of the reciprocal lattice and after that it simply repeat itself.

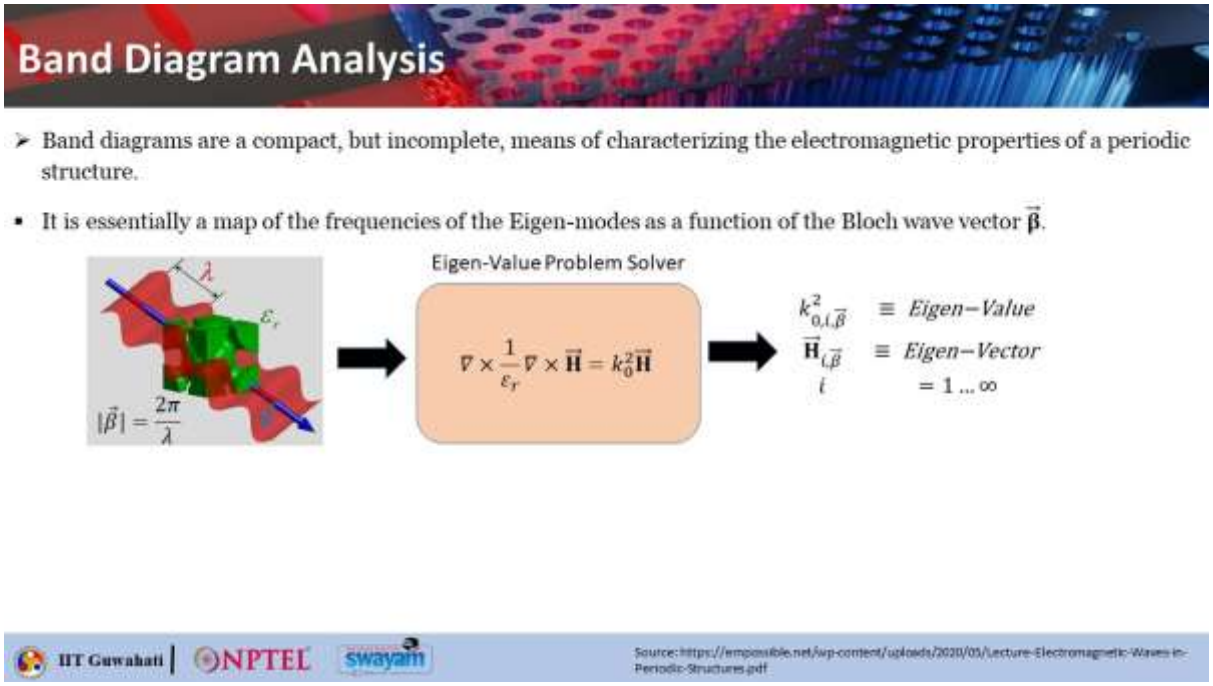



Now let us compare the wave equation in a semiconductor and in a photonic crystal, right.

So, due to the analogy between the Schrodinger equation and the wave equation, it seems that you can control electromagnetic wave inside periodic lattice like we can control electrons in semiconductors, right. here is how Schrodinger's equation look like and this is how wave equation looks like. So, here you can see psi r is basically a scalar wave function ok. H omega r is basically magnetic field component of the EM wave okay and we will discuss in the subsequent lecture that why we prefer to work with magnetic field component other than electric field components right. So, if you use Schrodinger's equation and from this eigenvalue equation you can try to obtain value of energy which is basically supported in this particular crystal semiconductor crystal and you can obtain the electronic band structure.

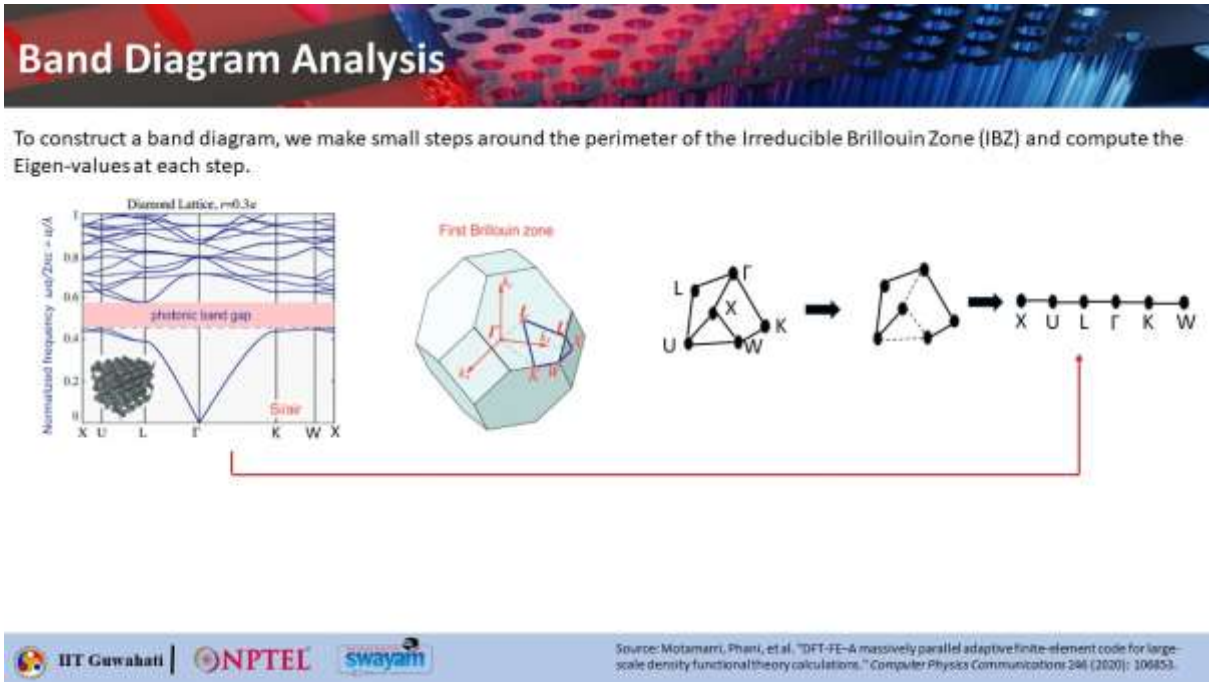
And the same exercise you can do for the photonic crystal and if you consider a square lattice like this, you can obtain a band gap. So here also you can get a band gap. And you can see that this is the band gap between the first and the second bands. You can also have some higher order band gaps. Here also you can see this is the band gap between first and second order.

bands and then you know you can also have higher order bandgaps. So, what is important here is to see that we this is for the square lattice this square pattern with k values ranging from minus pi by a to pi by a give you a square Brillouin zone. But out of symmetry you can only work with this one this triangular region and go across you know the points like gamma, x, m and gamma and that can give you the entire band structure. So, we will discuss this in details into this lecture okay in the subsequent slides.




So, band diagram analysis right. So, band diagrams are a compact but incomplete means of characterizing the electromagnetic properties of A. periodic structure, right. So, it is essentially a map of the frequencies of the eigenmodes as a function of the block wave vector beta. So, if you consider this, okay, it tells you that there is a crystal, periodic crystal which has got a permittivity of epsilon r, okay and the wavelength is lambda.

in this particular medium okay. So, what do you have this block wave vector okay. So, wave number the modulus of the wave vector gives you the wave number that is 2 pi by lambda right. So, the eigenvalue problem solver can be written as you know the equation can be written as $\nabla \times \frac{1}{\varepsilon_r} \nabla \times \vec{\mathbf{H}} - \kappa_0 \vec{\mathbf{H}}$ . $k^2_{0,i,\vec{\mu}}$ that is this gives you the eigenvalue and this is the eigenvector and i can be any integer. So, in order to construct a band diagram we make small steps around the perimeter of the irreducible Brillouin zone and then compute the eigenvalues at each step.

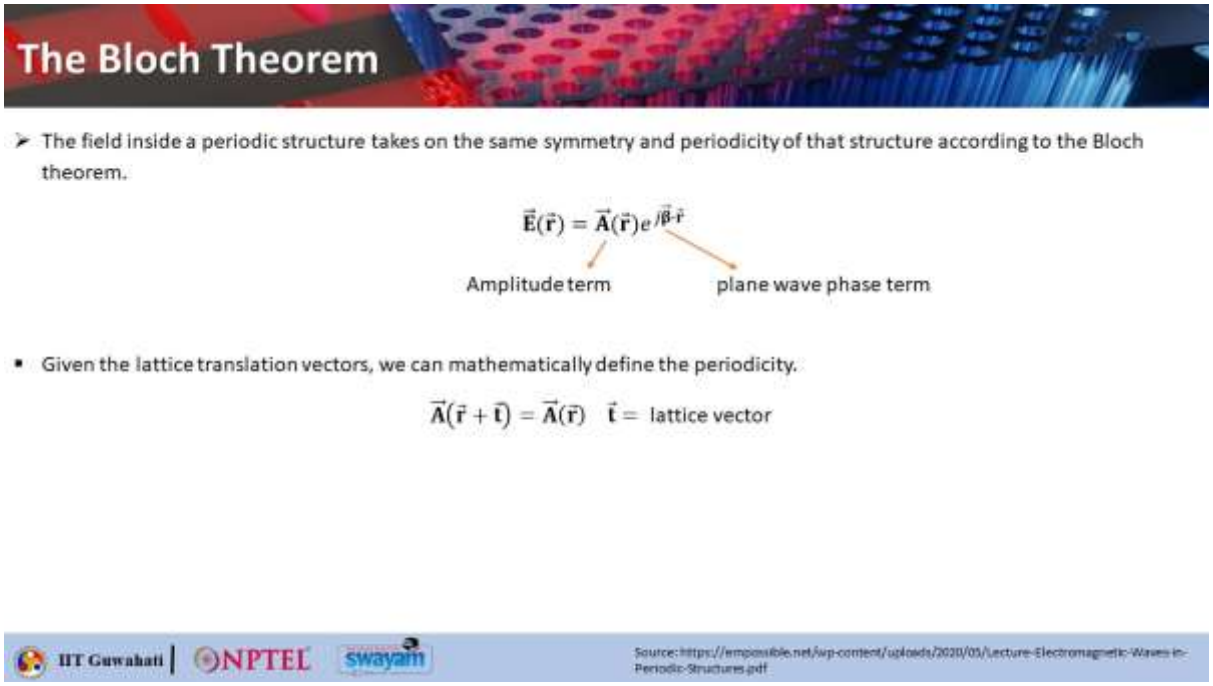



So if you take this 3d photonic crystal okay which is basically fcc lattice or a diamond lattice so this is the first brilliant zone of an fcc lattice and you can see that you can start from point uh so what are these uh kx, ky, and kz, these are basically the primitive reciprocal lattice vectors. And these are the important points along the periphery of the irreducible Brillouin zone. So here you can see you can start from x, then you move to u, then you move to l, then you move to gamma, then you move to k, then w and then back to x. So that is how you are basically traversing this entire brilliant zone, irreducible brilliant zone along its boundary. So anything in between you are actually calculating in between this all these directions are basically covered.

So these are all telling about the different directions of the wave factor okay fine. So that way you are actually looking for solutions of which frequency of the eigen function or you can say eigen mode satisfy this that equation right. So you can find you can see here that there is a photonic band gap. obtained.

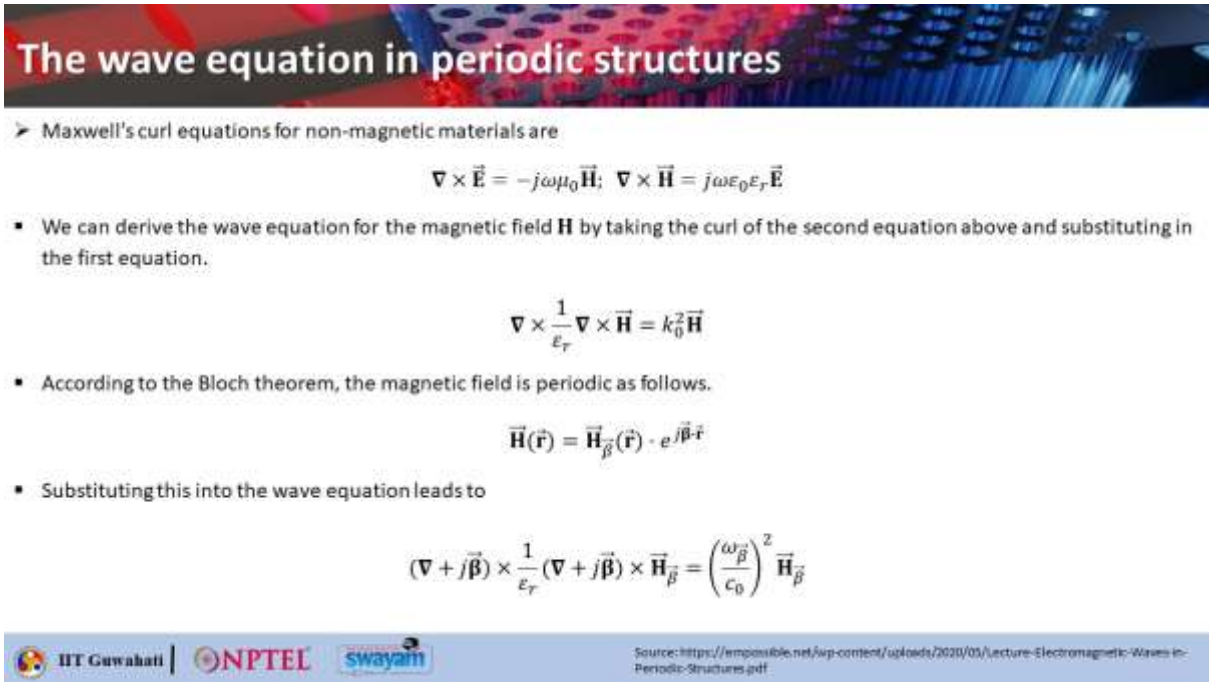
So, this is what has been explained clearly. So, you take out this particular irreducible brilliance zone and then you walk around the periphery you will get this particular sequence. So, it is not that you need to start with x and end with x you can start traversing from u also and then take make sure you go through all the points and come back to u that will also be fine. So, it is just a choice

# Band structure Engineering

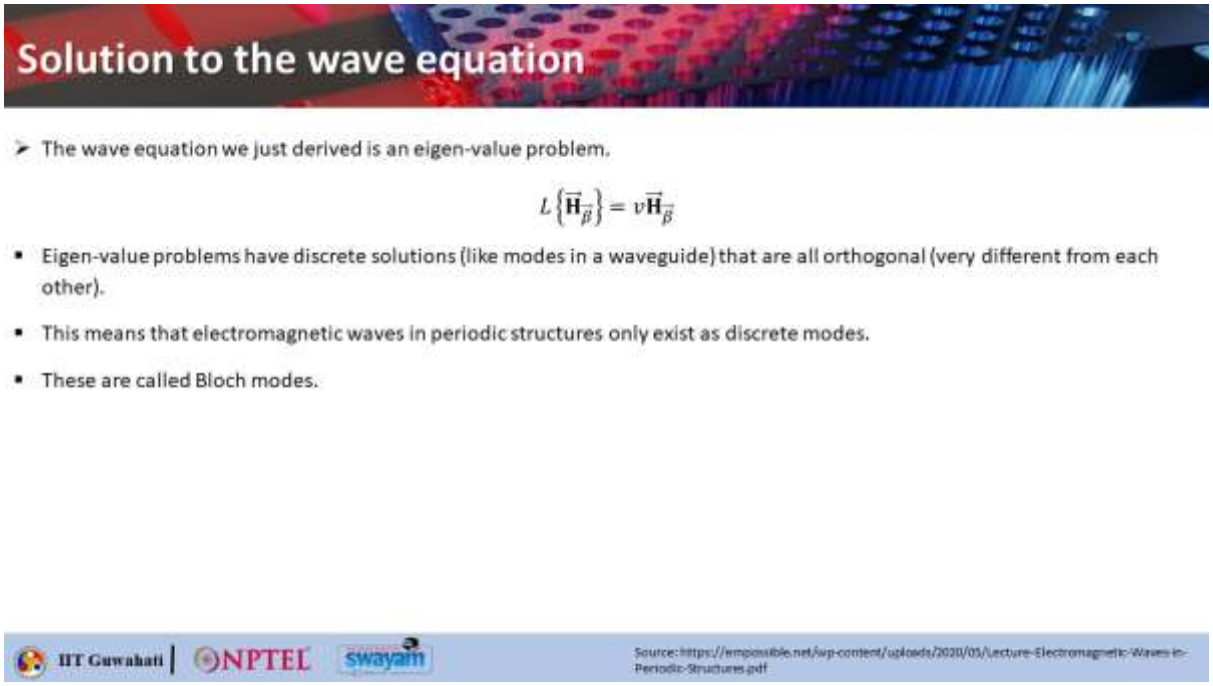



Now let us look into bench structure engineering. So, when you work with bench structure engineering block theorem is a very important mechanism to understand how it works okay.

So, the field inside a periodic structure basically takes on the same symmetry and periodicity of that of the structure according to the block theorem right. So, we understood that $\vec{E}(\vec{r})$, the electric field okay will have an amplitude term and then you have this phase term which is given by $e^{j\vec{\beta}\cdot\vec{r}}$. Given the lattice translation vectors, we can mathematically define periodicity. So, you can say this amplitude term is basically showing periodicity as $\vec{A}(\vec{r}+\vec{t}) = \vec{A}(\vec{r})$, where $\vec{t}$ is your lattice vector.

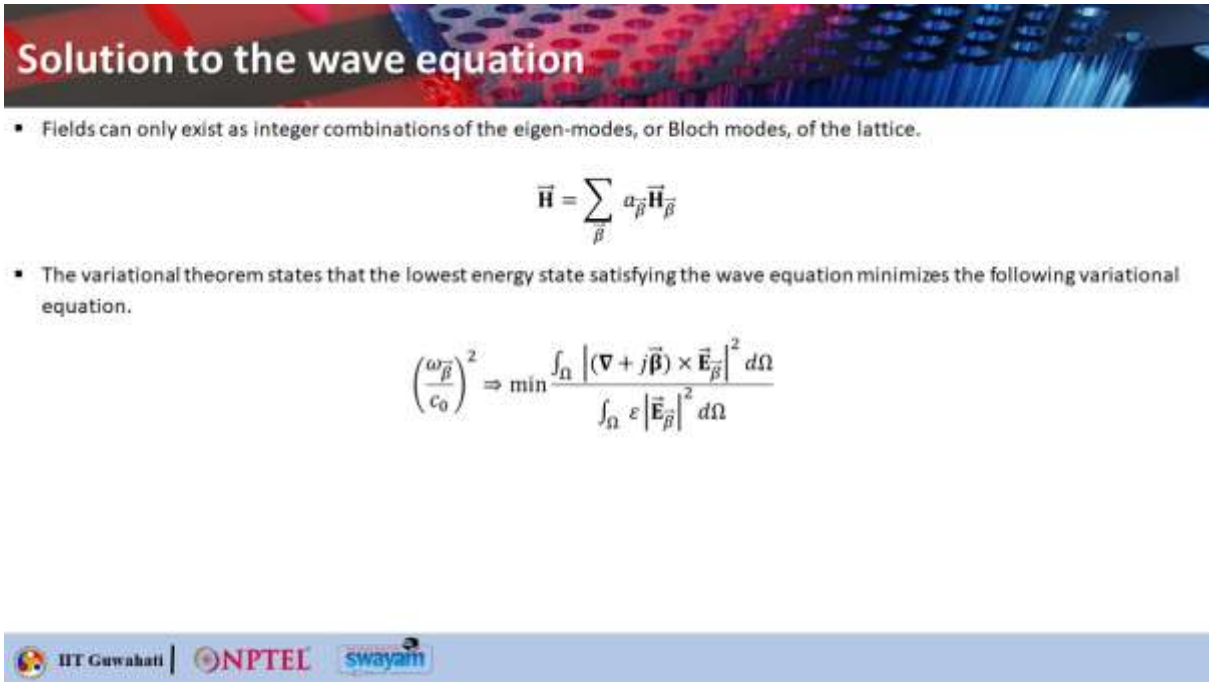



So, Maxwell's curl equation for non-magnetic medium you can pick this up from the initial discussion. So, what you can do you can replace this magnetic field by the electric field okay in the first equation and then you can obtain the So, what you can do you can derive the wave equation for the magnetic field by taking curl of the second equation. So, it will become curl of curl of H will be equal to this constant time curl of E and instead of curl of E you can do the substitution from the first equation and you will get something like this. So, according to the block theorem the magnetic field is periodic as it follows this particular form. So, you can write hr equals $\vec{\mathbf{H}}(\vec{\ }, \vec{\ }$ .




So, if you substitute this particular form into the wave equation that you have seen you will obtain this particular equation. So, what is this? So, the wave equation what we have just seen is basically eigenvalue equation. It is something like you know L is a wave equation operator that is working on this field magnetic field and giving you a scalar time the field again. So, this is basically you know the eigenvalue.

right. So, eigenvalue problems have discrete solutions something like modes in waveguides that are all orthogonal right. It means they are very different to each other and this means that you know the solutions of electromagnetic waves in periodic structure also exist as discrete modes and they will be called as block modes. Now the fields can exist as also linear combination of the different eigen modes or block modes of the lattice. So, you can think of $\vec{\mathbf{h}} - \sum_{\mu} \vec{\ }_{j}$. It means you know you can have this different linear combination also forming a block mode which is supported in that particular crystal.

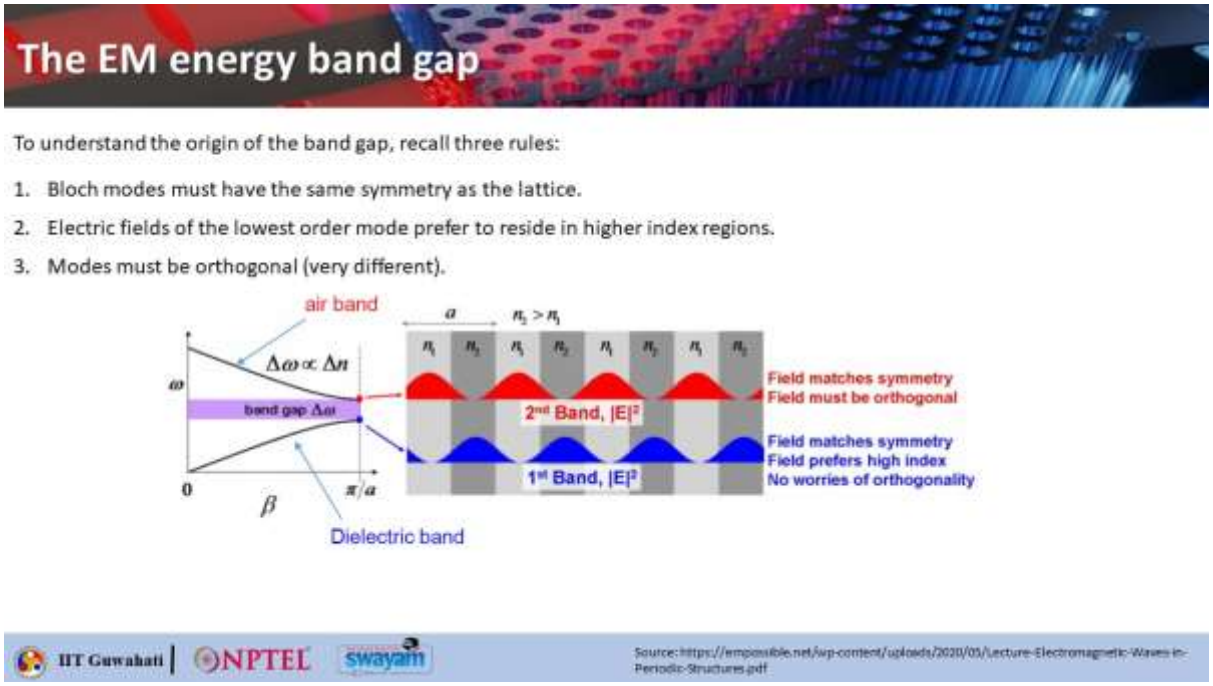





Now, the variational theorem states that the lowest energy state satisfying the wave equation minimizes the following variational equation okay. So, $\left(\frac{\omega_{\vec{\nu}}}{c_0}\right)^2$ it can be written as

$\min \frac{\int_\Omega \left|(\nabla + j\vec{\boldsymbol{\beta}}) \times \vec{\mathbf{E}}_{\vec{\nu}}\right|^2 d\Omega}{\int_\Omega \varepsilon \left|\vec{\mathbf{E}}_{\vec{\nu}}\right|^2 d\Omega}$ — okay. So, to minimize this equation what you have to do your your best just looking for minimum of this equation right. So, to minimize this you need to maximize the denominator of this equation. So, denominator of this equation has got permittivity and the intensity of the electric field right it is basically E square right.

So, this would happen when most intense field will reside in the high permittivity region. So, you can have you know this product to be very large as compared to you know if this is small this product will go small. So, what do you want your field to be more mostly concentrated in the high permittivity region and that is how the field of the lowest order prefers to be in the high permittivity region and we can see that later on

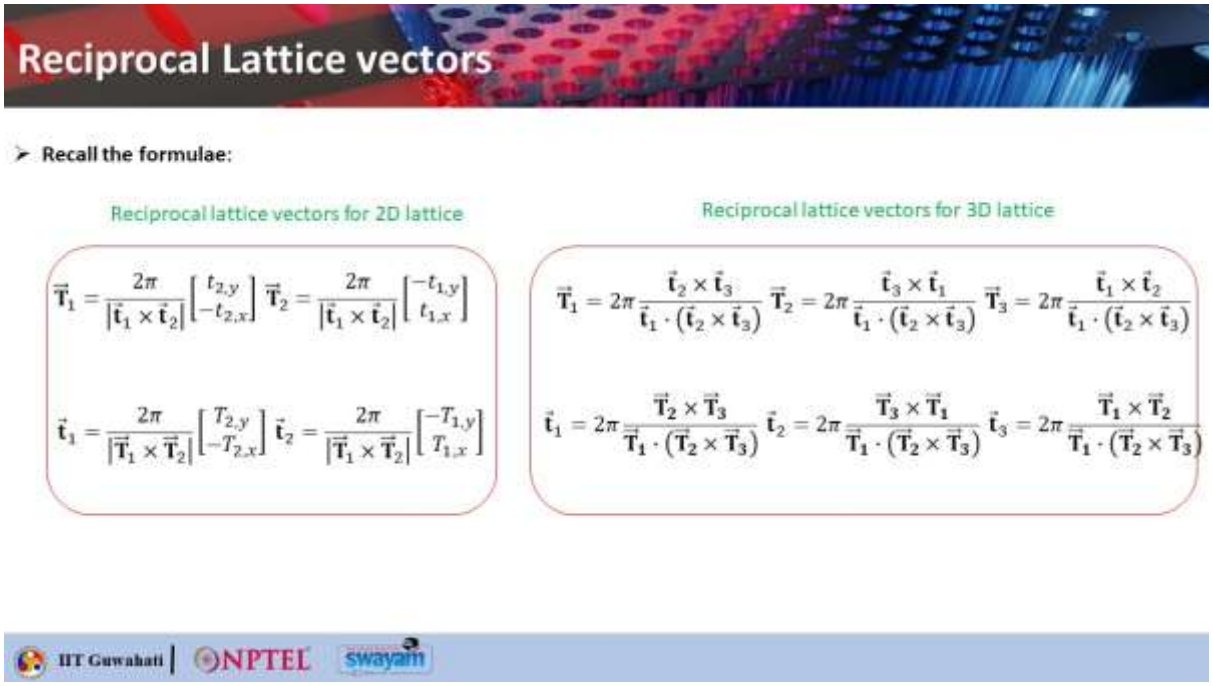



So, to understand why we get bandgap you just recall three important rules. The first one is that the block modes must have the symmetry Same as the lattice.

Second rule is that electric fields of the lowest order would prefer to reside inside the higher index region. And the third one is that modes must be orthogonal. So, they should look very different. So, if you see this particular band diagram okay, so this particular mode is the mode of the lowest order and it prefers to be in the you know higher dielectric constant material. So, if you think of the periodic crystal having two different dielectric constant n1 and n2 by convention the darker region is higher refractive index.

So, it is n2 is greater than n1 and this n1 plus n2 thickness this thickness is got gives you the periodicity A and that is only repeated ok. So, the first thing the block modes must have the same symmetry as the lattice yes it does ok. Then you satisfy this one ok that the electric field of the lowest order should be here and then you have to see that the modes must be orthogonal. So, in that case, you got to have the modes. The second mode should be having peak in the lower refractive index region.

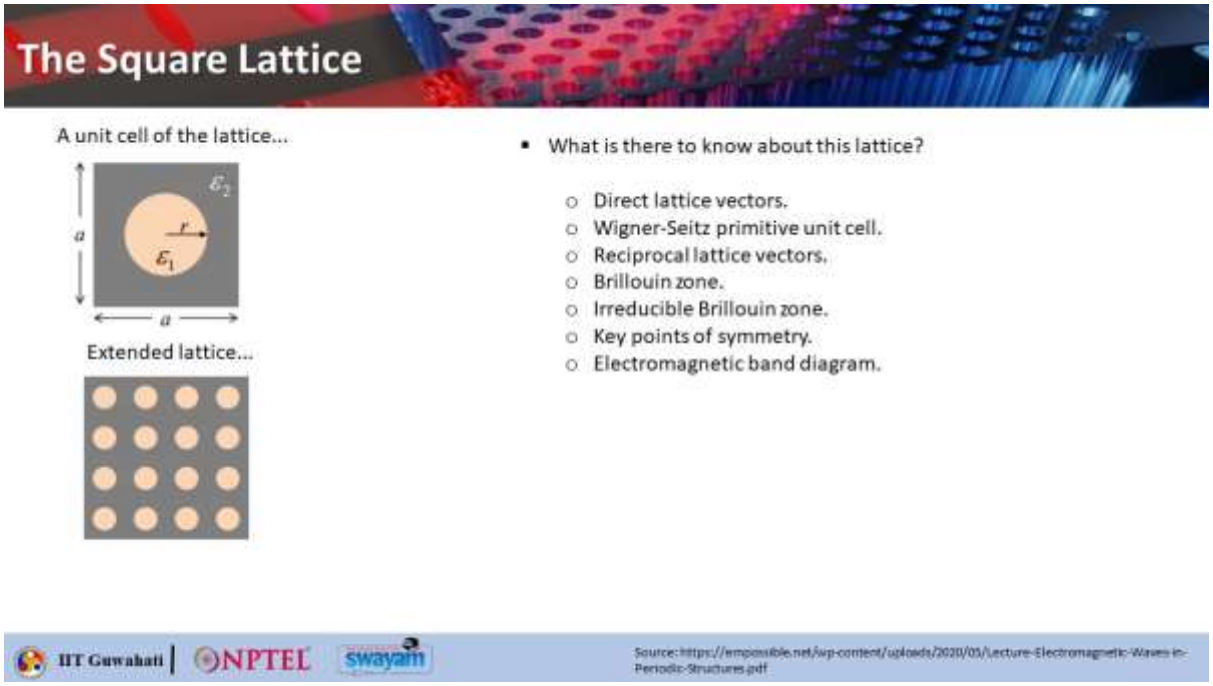
So this is important because if you have two modes with the same periodicity, but different effective index then only it is possible that they are of different omega right. So, they are having same you know beta, but they are having different omega. So, that is how you can see that the second band okay will have this kind of a profile




So, now let us look into the calculations of reciprocal lattice vector. So, if you recall the formula that you have seen in the last lecture.

So, if you take a 2D lattice you can consider the know reciprocal lattice vectors to be capital T1 and capital T2 and the direct lattice vectors or real lattice vectors to be small t1 and small t2. So, this is how you can actually calculate capital T1 and capital T2 from small t1 and small t2 and vice versa. The same thing can be extended to you know 3D lattice. So, here in reciprocal space you will have three primitive lattice vectors which is capital T1, capital T2 and capital T3 and you can calculate them from the direct primitive lattice vectors or you can say primitive lattice vectors of the direct lattice small t1, small t2 and small t3 using this formula and you can do the reverse operation as well. So, with the value of real and reciprocal lattice vectors and their you know interchangeability you can understand that you if you know the information of one lattice you can always interpret the other lattice right

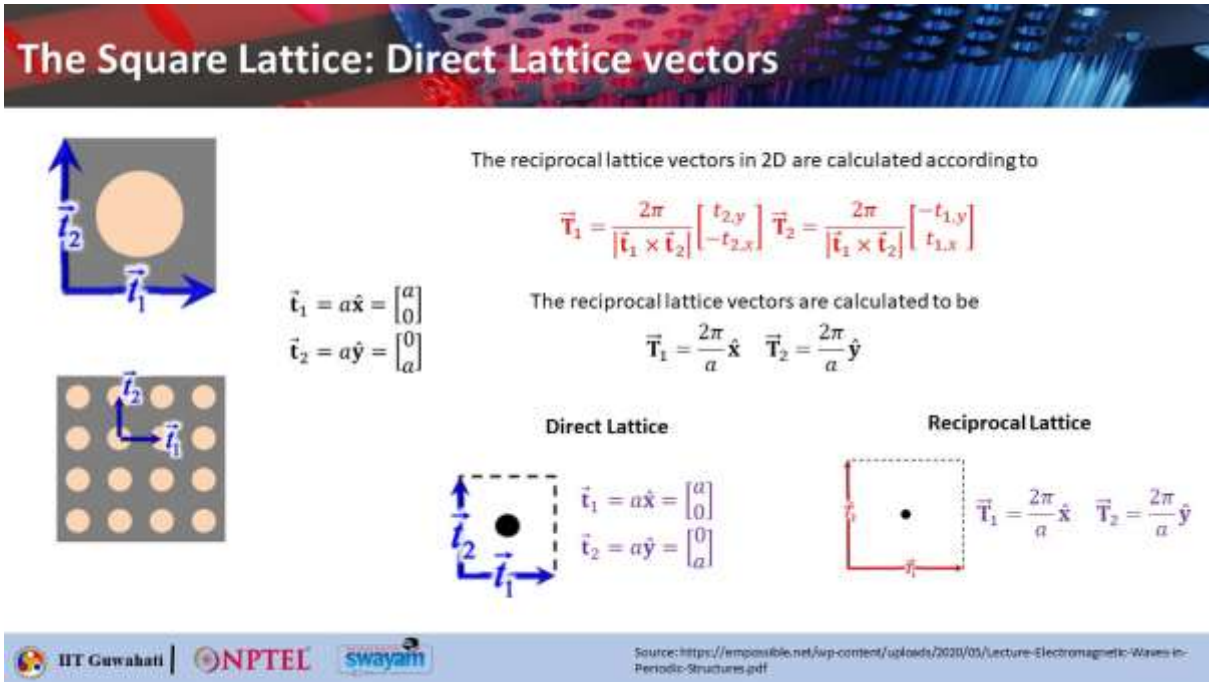
# Band structure Analysis of standard lattices




So now let us look into band structure analysis of standard lattices. let us first consider a square lattice. So, this is basically the unit cell of a square lattice. So, what is this lattice you can think of a beautiful dielectric cylinder okay of epsilon 1 permittivity okay.

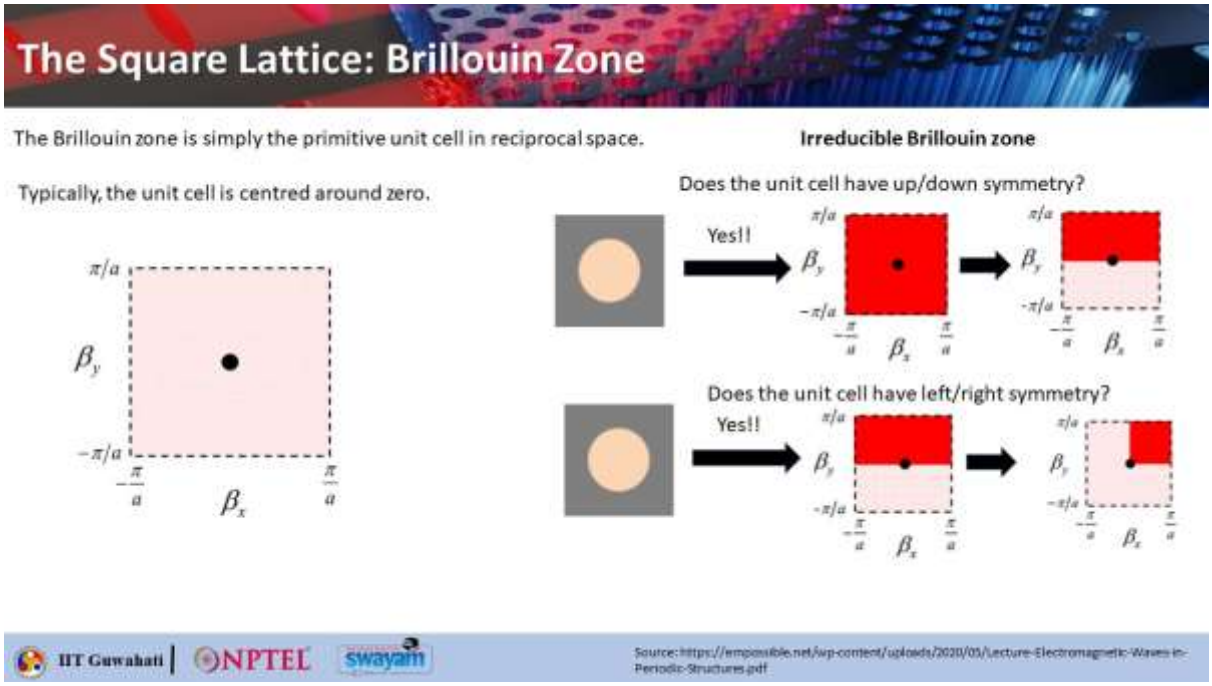
and the neighboring region is air. But as I told you by convention, you can think of the darker region to be the material and material of higher refractive index. So, in that case, you can consider this as a cylindrical hole, which is air, and this is your material. So, if you take this square unit cell, which is having dimension of a, So, and repeat it periodically you basically get this particular square lattice of cylindrical holes. Now, because it is a 2D lattice you can only think of you know as circular holes. So, what is there to know about this lattice? First, we need to find out the direct lattice vectors, then we need to obtain what is the Wigner stage primitive unit cell in this case which is repeated periodically to create this direct lattice.

Then we should obtain the reciprocal lattice vectors, identify the Brillouin zone in which we should be able to find out what is our irreducible Brillouin zone. and mark those key points of symmetry and finally obtain the electromagnetic bank diagram. So, that is how you will be able to analyze a periodic structure completely. So, now let us begin with identifying the direct lattice vectors.



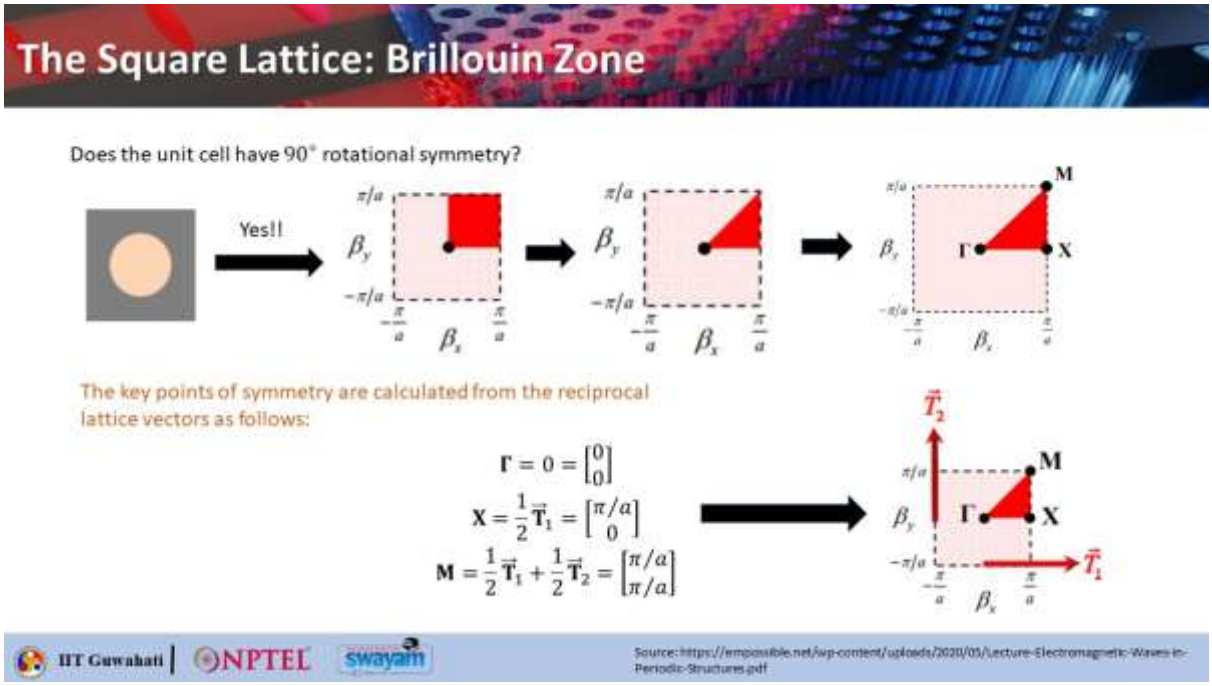

So, you can consider t 1 and t 2 as your direct lattice vectors. So, t 1 is basically $\vec{t}_1 - a\mathbf{x}$ or you can write as $\begin{bmatrix} a \\ 0 \end{bmatrix}$ and t 2 is nothing but $\vec{t}_2 - a\mathbf{y}$ . So, you can write it as $\begin{bmatrix} 0 \\ a \end{bmatrix}$. So, this is how t 1 and t 2 are marked in the original lattice. So, using that information you have these equations okay that can help you calculate the reciprocal lattice factors capital T1 and capital T2. So once you put them into place you will find that capital T1 is $\vec{T}_1 - \frac{}{a}\mathbf{x}$ and capital T2 is $\vec{T}_2 - \frac{}{a}\mathbf{y}$ .

okay. So, one more time to put them side by side this is how our direct lattice vectors look like and this is how our reciprocal lattice vectors look like.



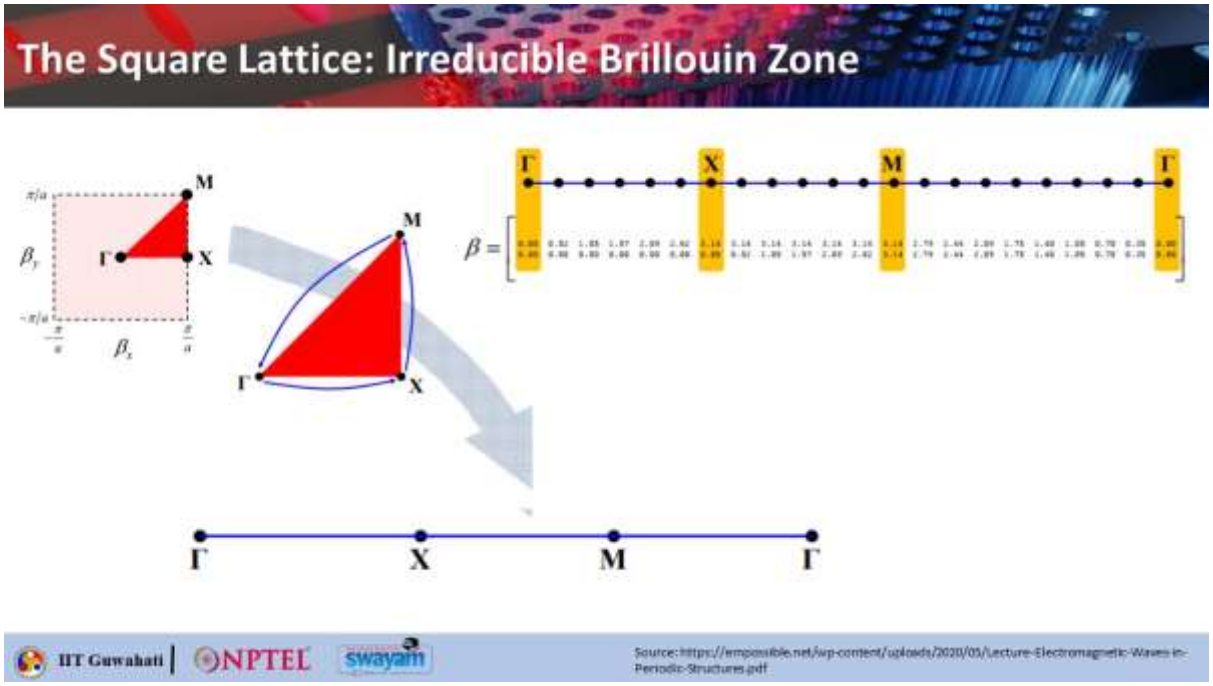

Now, so the Brillouin zone okay. So, the Brillouin zone is basically the primitive unit cell in reciprocal lattice. So, typically the unit cell is centred around 0. So, you can write instead of having you know 2 pi by a you can 0 to 2 pi by a you can make it symmetrical from minus pi by a to plus pi by a okay for beta x that is along the x direction you can write and for beta y you can also write minus pi by a to pi by a.

So, how do you find out the irreducible Brillouin zone in this case? So, first question you will ask, does the unit cell have up-down symmetry? The answer is yes. So, it has got up-down symmetry and you can say the upper part is same as the lower part. The next question will be, does the cell unit cell have left right symmetry? The answer is again yes ok. So, I think it has to be tilted the left right symmetry is like this ok. So, it should be red painted here ok, it should be painted here ok and not here.




So, you understand right this is left right symmetry. So if you say that you can only take this particular region okay and think of that okay if I have only this quarter information using left right symmetry and up down symmetry I will be able to recreate the entire brilliant zone yes. Now the last question that we will ask that does the unit cell have 90 degree rotational symmetry? Now if you rotate this unit cell by 90 degree does it look same? The answer is yes and if so then you can only use this half of this particular area and then use the rotational symmetry to combine it. So, this becomes your irreducible Brillouin zone. So, first you will get this irreducible Brillouin zone, you will use the rotational symmetry and then you will use left right symmetry and then you will use up down symmetry to get the complete square Brillouin zone.

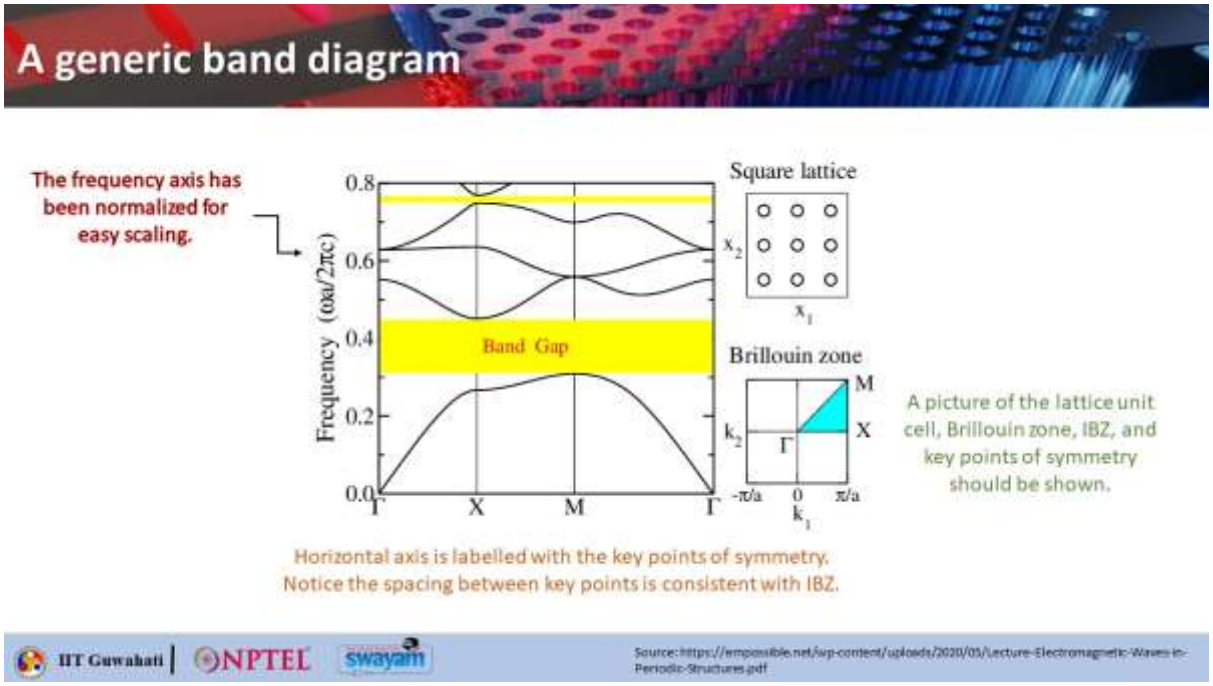
fine. So, now let us identify the key points of symmetry which can be calculated from the reciprocal lattice vector. So, gamma is always at the center. So, you mark it as $\Gamma = 0$ you can write it as $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$. x is at the middle of one of the edge okay so x is basically $\mathbf{X} = \frac{1}{2}\vec{a}_1$ so that is $\begin{bmatrix} \pi/a \\ 0 \end{bmatrix}$ and this is at the corner point so you go half this way and half this way so it is basically $\mathbf{M} = \frac{1}{2}\vec{a}_1 + \frac{1}{2}\vec{a}_2$ so you can write this point as you know $\begin{bmatrix} \pi/a \\ \pi/a \end{bmatrix}$ right. So, this is how you can express the key points of symmetry of the irreducible brilliant zone of a square lattice.




Fine. So this is what we understood. This entire square is basically the reciprocal lattice. This red highlighted triangle is basically the irreducible brilliant zone. And then if you want to cover all the points here in this, you have to move around the periphery of this and come back to the same point. So you can start with gamma. then you go to x then you go to m and then come back to gamma like this okay so this way you come back to gamma so here also you see what you are doing you are basically having your gamma is basically beta 0 0 x is basically pi by a comma 0 so a is been taken as 1 ok.

This is pi by a comma pi by a and then you get back to 0. So, in between you can have all these different values ok. So, that tells you about you know how you move around. So, from here to here ok. So, what is y is 0 ok and you can improve you can take different values of now this and go from 0 to 3.

Once you have reached this point okay your y value is fixed sorry the x value is fixed the y value will change. So, 3.14 here remains same only the y value will change and that should also change from 0 to 3 in different steps. So, these are the steps you have taken. ok and when you go from here to here ok you are basically at 3.14 3.14 that is x coordinate y coordinate ok from here you have to go to 0 and 0. So, you can determine the steps in which you want to go and then these are the different points of beta for which you will be calculating the band structure. So, you can take more finer points or less number of points okay depending on your calculation fineness that you require to get a smooth line okay.

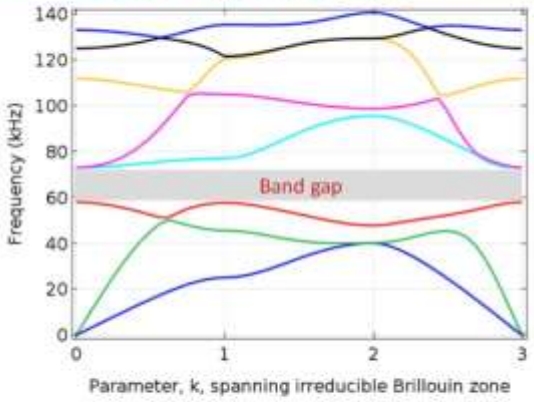



So, this is the band diagram that you will obtain once you calculate for all these different values of beta ok. So, this we have already seen in the initial slides. So, here one thing to note is that you are using frequency which is normalized. So, this is basically A by lambda. So, that helps you in finding out if you have a given wavelength you can actually find out the required lattice constant of the square lattice to obtain this kind of a band gap.

Right? Okay. So we understood how we construct band diagrams. So this is basically nothing but in the x-axis you have nothing but the wave vector beta or k that is spanning across the irreducible Brillouin zone. And here you calculate the frequency of those modes which can satisfy that wave equation right. So, few places there are no solutions means for this particular frequencies there is no solution to the wave equation it means wave for those frequencies cannot propagate through the crystal and that is what is the band gap or the forbidden bands. Now, how do you get complete band gap? Okay, so what you have seen here is that you know this is the full brilliant zone in two dimension. So, beta x, beta x and beta y okay and this is how you know if you try to visualize that this is the first band okay.

Then this is the second band, this is the third band okay. This is how where you have your you have got your normalized frequency right.

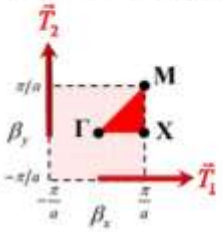
## Constructing the Electromagnetic Band Diagram

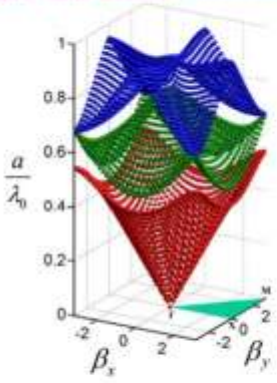





## The Complete Band Diagram

The Full Brillouin Zone for 2D lattice



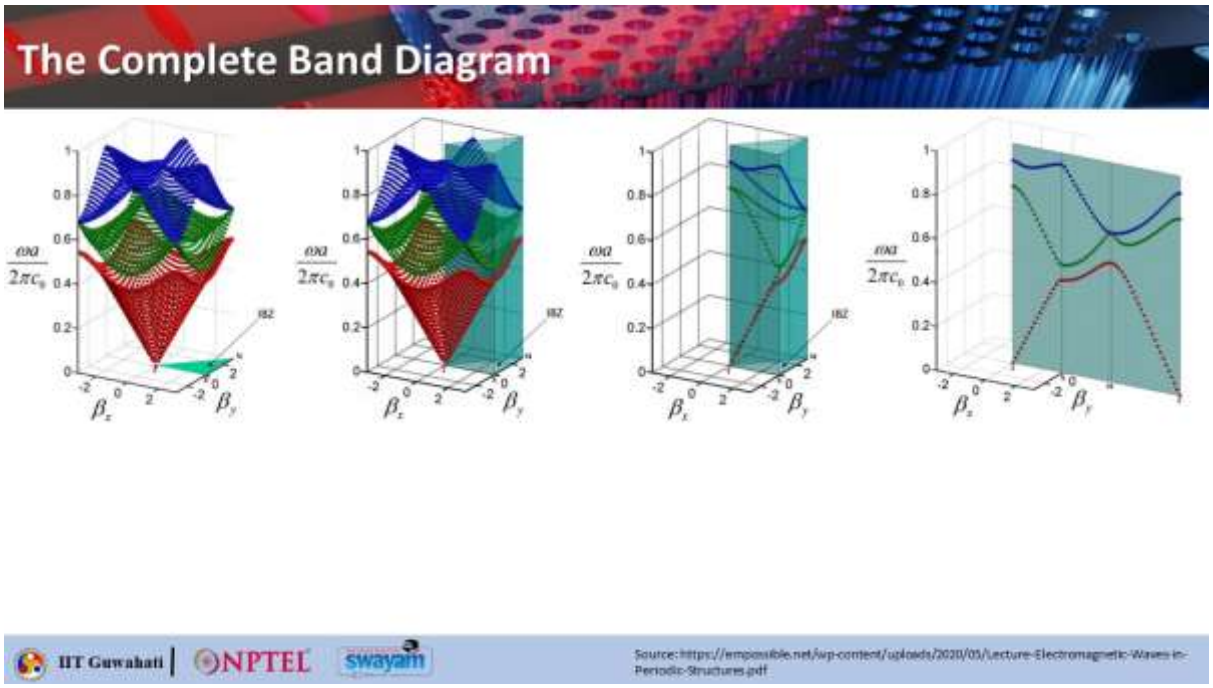





So to visualize the relation between complete banding diagram and in a band diagram. we will start with the complete band diagram first ok. So, this is a complete band diagram right and then we consider this irreducible Brillouin zone and then vertically extend them as walls ok and we will actually try to focus on. So, this is the complete band diagram and then once we have raised these

walls we will try to see the cross section of these bands with those walls.

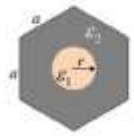
So, this is how the bands will intersect with this band diagram or bands this wall will interact and then if you open up this irreducible Brillouin zone ok. So, you can continue gamma x and m. So, you have gamma x m and gamma.




So, when you open it up. So, this is what we see as the band diagram. right so this is the complete band diagram okay and this is the band diagram that we see to describe things right so i hope it is uh easy to understand okay so this ordinary band diagram typically tells you all the story okay however dealing with this kind of diagram or drawing it is not very straightforward. So, if you only deal with the band diagram in the irreducible brilliance zone that will give you the complete information about the lattice.

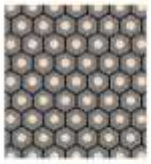
## The Hexagonal Lattice

A unit cell of the lattice



$r = 0.35a$
$\varepsilon_1 = 1.0$
$\varepsilon_2 = 9.0$

Extended lattice...



- What is there to know about this lattice?
  - Direct lattice vectors.
  - Wigner-Seitz primitive unit cell.
  - Reciprocal lattice vectors.
  - Brillouin zone.
  - Irreducible Brillouin zone.
  - Key points of symmetry.
  - Electromagnetic band diagram.



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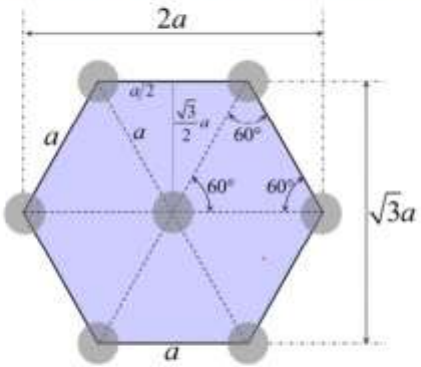
We will take another example here let us consider a hexagonal lattice. So, this is the unit cell here again you have a cylindrical hole, but this time the unit cell is a hexagonal structure.

So, the radius is 0.35a that is also you know is a lattice period. So, this is normalized. So, epsilon 1 is 1. So, that is air and this is some material which has got a dielectric constant of 9 and this is how the extended lattice looks like. So, again we will try to see all these different points in this case. So, first of all let us consider this geometry of the hexagonal lattice.

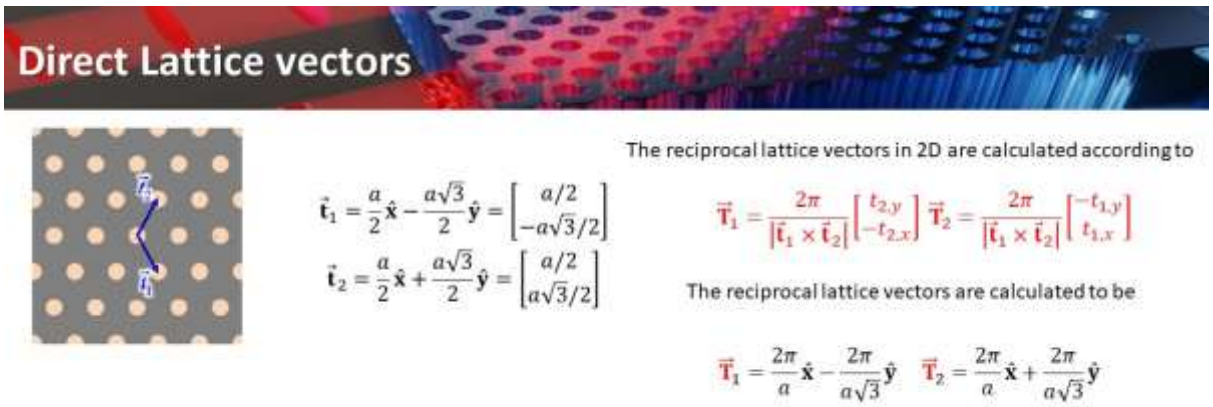
## Geometry of the Hexagonal Lattice






So, in hexagonal lattice each side is a. So, if you take the distance from this point to this point that is basically 2a. However, the distance point from this point to this point is root 3a right. So, you can

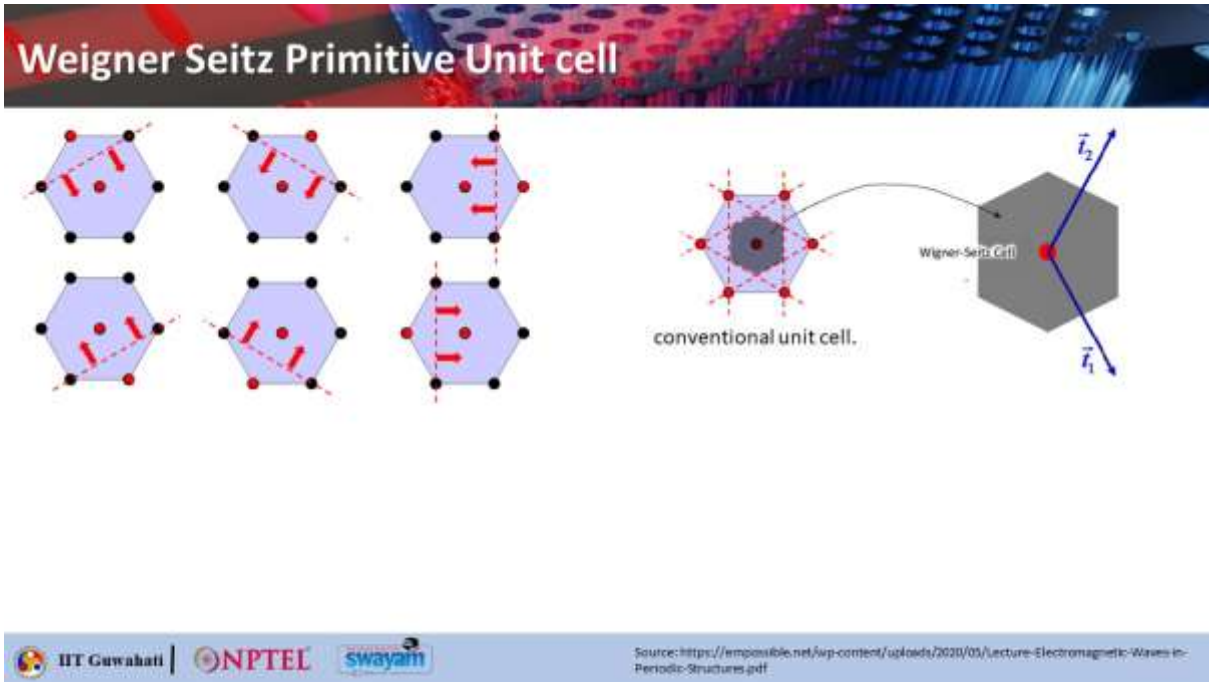
actually calculate this it is very simple because the angle it they make between to this point and this point is 60 degree. So, you can actually do basic geometry and find out these distances.




So, if you consider the direct lattice vector. So, in this case these are the direct lattice vectors t1 and t2. So, t1 can be written as a by $\vec{t}_1 - \frac{a}{2}\hat{x} - \frac{a\sqrt{3}}{2}\hat{y} = \begin{bmatrix} a/2 \\ -a\sqrt{3}/2 \end{bmatrix}$. So, this you can see from here also. So, T1 is basically marked like this.

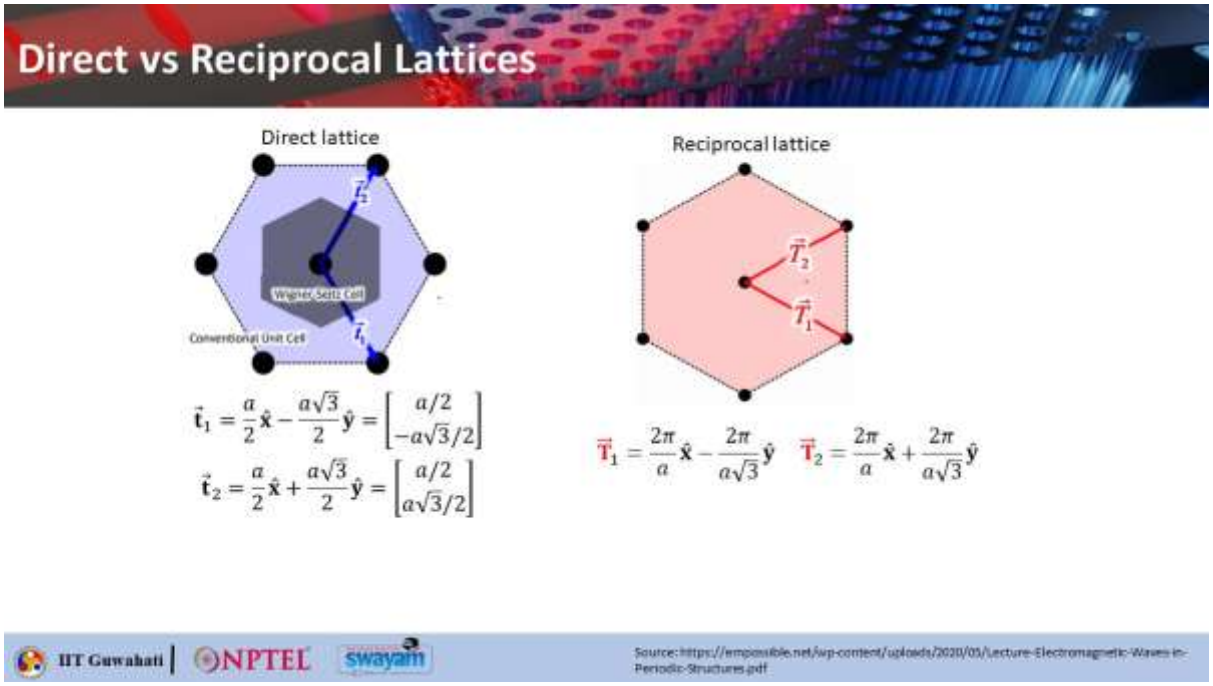
So, it is halfway here which is $\vec{T}_1 - \frac{2\pi}{a}\hat{x} - \frac{2\pi}{a\sqrt{3}}\hat{y}$ okay. Similarly, T2 is $\vec{T}_2 - \frac{2\pi}{a}\hat{x} + \frac{2\pi}{a\sqrt{3}}\hat{y}$. So, once you have known small t1 and small t2, you can use this formula and calculate capital T1 and T2 straightforwardly okay. So, capital T1 and T2 comes out to be this.

$\vec{T}_1 - \frac{2\pi}{a}\hat{x} - \frac{2\pi}{a\sqrt{3}}\hat{y}$ $\vec{T}_2 - \frac{2\pi}{a}\hat{x} + \frac{2\pi}{a\sqrt{3}}\hat{y}$ okay. So, the primitive translation vectors or the direct lattice vectors are basically the ones that connect the two adjacent sides, okay. And all sites in this lattice should be reachable through some kind of you know integer combination of this lattice vectors. Something like if you want to reach to this particular site it simply you know from here you can extend it right. If you want to go to this one you have to go like this and then you can extend this one and you can go to this particular site and so on.



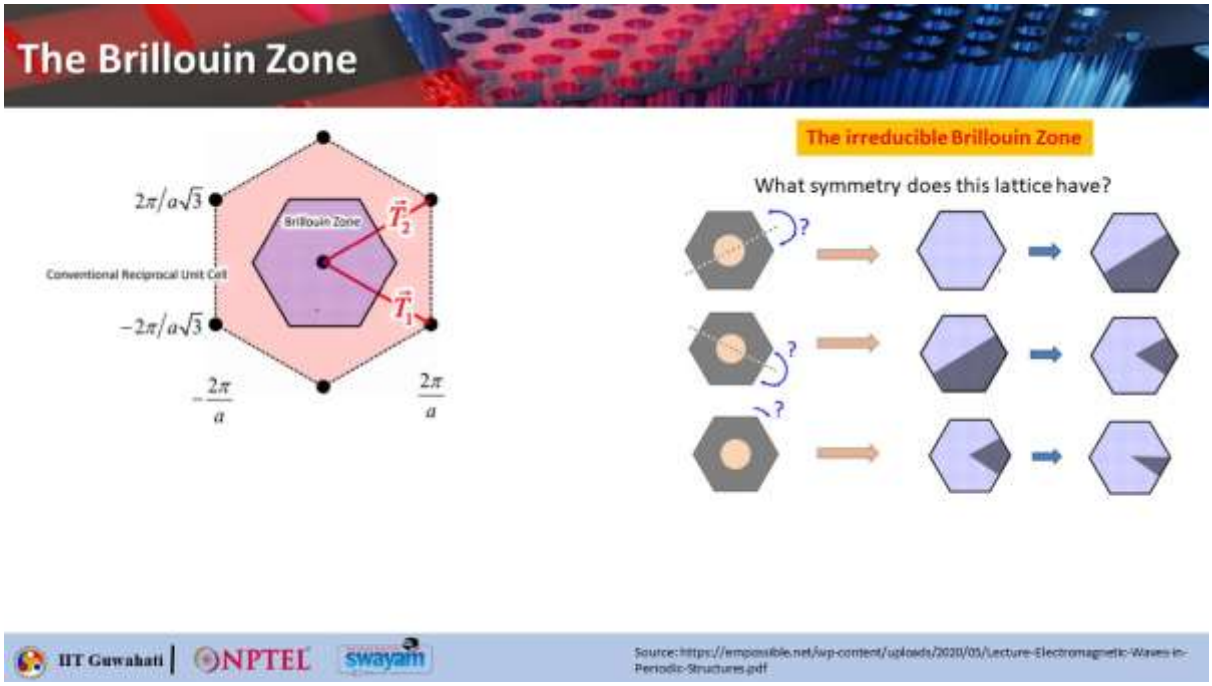

So, we will see here the Wigner state primitive unit cell calculation which you skipped in the square one because we have already discussed once.

So, here you can see that this is the direct lattice and the unit cell is a hexagonal. So, if you consider these two points okay and you are mainly focusing on the center point lattice point so if you take these two points and then draw this particular line that bisects the region so anything that falls within this area I will use the laser so anything that falls within this area is actually closer to this point similarly when you consider this lattice point and this one so this is the center point so if you draw this line so anything within this side of the line is closer to this point than this point right and you repeat this exercise what you get is like So, you add up all these different areas. So, this, this, this, this, this and this, you will get a hexagonal unit cell inside and that is nothing but the Wigner's H cell.




And if you put the primitive lattice vectors there, so this is how T1 bar and T2 bar will looks like, okay. So, this is the direct lattice. okay so this is how so this is the conventional unit cell okay which we could have repeated to obtain the actual big lattice so these are all in real space or direct lattice from that you can actually calculate what is the wigner shade cell so if you repeat this cell also that will also give you the you know a periodic lattice so we have seen how to define the primitive that is vectors t1 and t2.

Similarly, you can also calculate, so this is the direct lattice, this is the reciprocal lattice

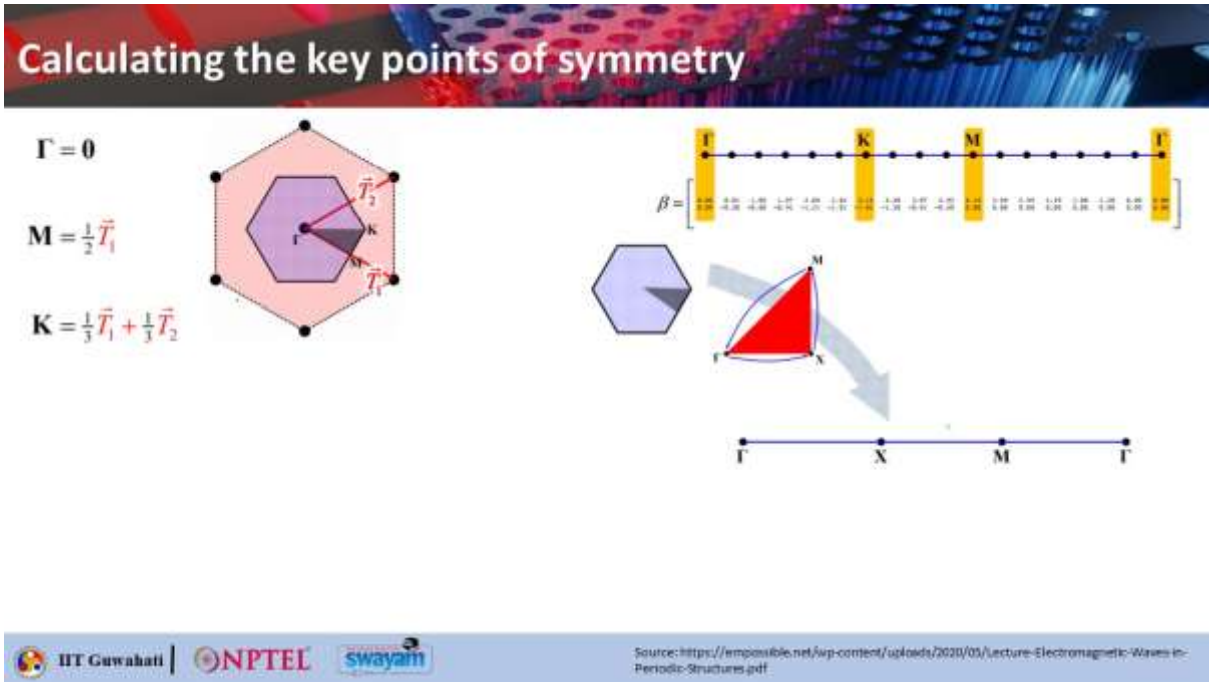



You have calculated what is capital T1 and capital T2 which are basically the reciprocal lattice vectors. And now in the reciprocal lattice, you can also do the same kind of calculation or method that you have done for Wegener stage cell and find out what is the Brillouin zone. Something like if you take this point and this point. So this line marks the area, this particular line will mark the area where the points here are basically closer to this one. Similarly, if you consider this point and this point, this particular line considers the region which is closer to this point and so on.

If you repeat it, you will get this particular hexagonal shape which is the Brillouin zone. So, this one is a conventional reciprocal lattice unit cell okay and these are the coordinates marked and this one is the irreducible this one is the Brillouin zone okay. From that we can also apply those concepts of rotational symmetry, up down symmetry and finally we can actually see that if you apply this symmetry that whether this part is symmetric to up and bottom? The answer is yes. So you can only consider one part.

And then you can consider whether these two parts are equivalent. The answer is yes. And then whether if you rotate it by 90 degree, it is okay.

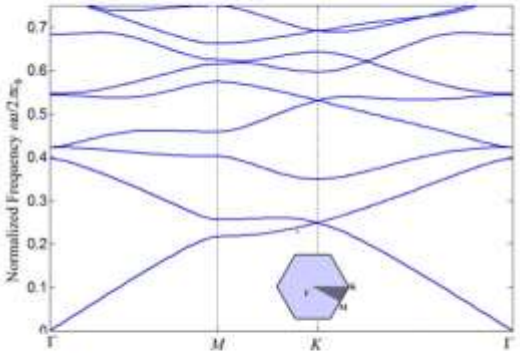
It is reproducing the same structure. The answer is okay. So you can only go for this kind of cell. Okay. So this becomes your irreducible Brillouin zone. Okay, so what we understood, let us mark. So, this bigger thing is the conventional unit cell of reciprocal lattice. The one here is basically the Brillouin zone and this one is the irreducible Brillouin zone for hexagonal lattice.




Now, let us mark those important points. So, gamma is the center, M1 is basically you can see it is half of T1 and k is basically one-third of T1 plus one-third of T2 and that will give you this k vector. So, once you have these three points gamma m and k gamma m k I think it is this particular figure is not correct ok. It should be gamma then say m. So, here it is it should be m ok. not x okay and this so what do you do you can actually don't you don't need to look into this one okay you can simply mark this as gamma this as m and this as k okay so you can and this will be gamma this is not x this will be m okay and this will be k right and this is gamma again.

So, you can start from gamma, gamma to m then to k and then back to gamma. So, you will have gamma m k gamma right. So, like this. So, do not look into this particular calculation this is I think by mistake I have repeated k, okay. So, if you do the calculation, you see that you get this is your band structure

# The final Band Diagram



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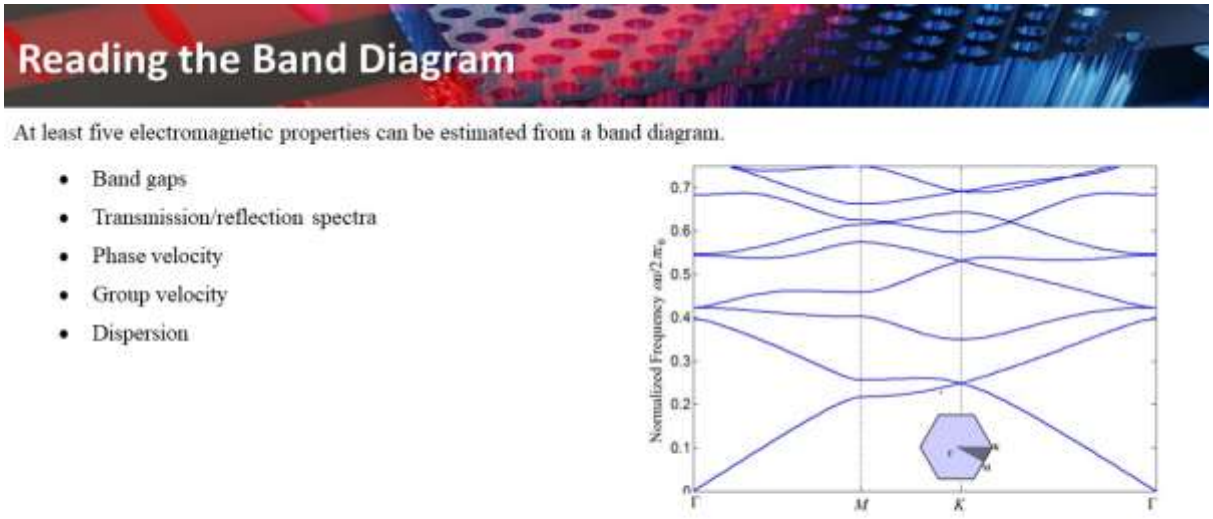
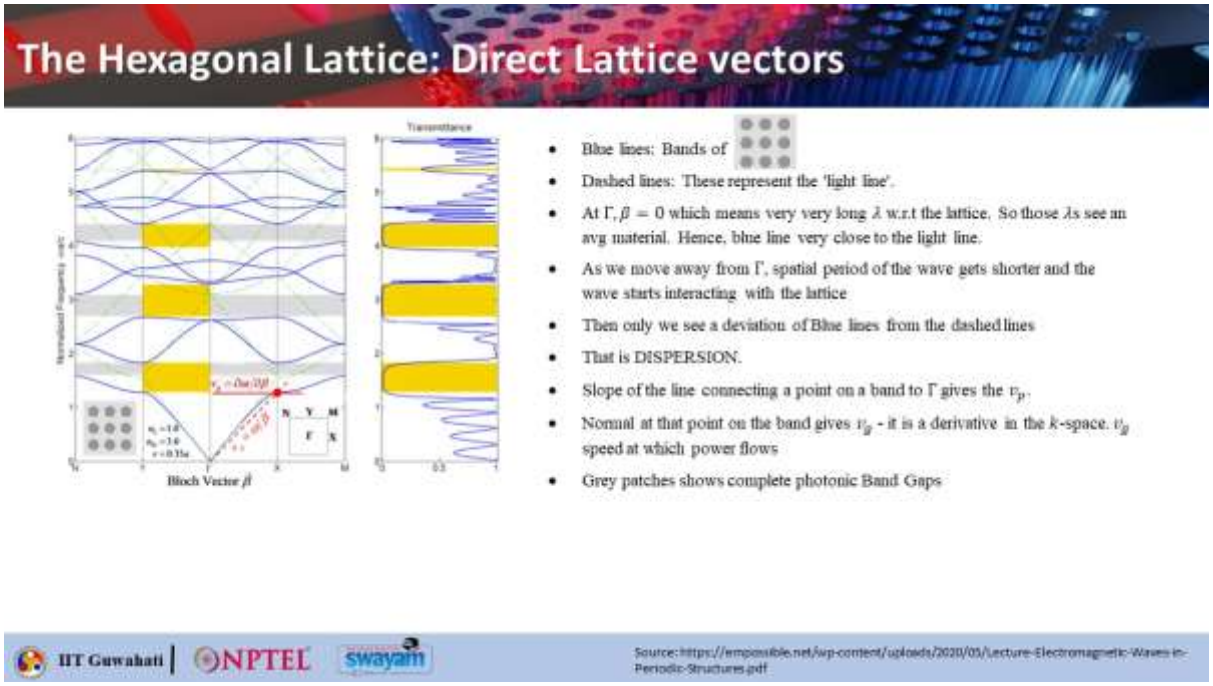



Now, this is the band diagram and what you can see here that at least you know 5 different electromagnetic properties can be estimated from a band diagram. First thing you can talk about the band gaps then you can based on the band gap you can also discuss about the transmission reflection spectrum.

You can discuss about the phase velocity, group velocity, dispersion and so on.




So, let us take one example. So, let us take this particular band diagram and try to read out the information. So, here you can see that we are basically considering a square array. And the darker region tells you that this is basically an array of dielectric cylinders with refractive index NH equals 3.

And the lighter region is having refractive index NL equals 1. And the radius of these cylinders are basically R equals 0.35A. So with this particular square array, you can actually calculate what is the points important points over here okay and n y gamma x m are the important points and you can see that you could have actually gone in only one side but it's fine it shows you the symmetry thing okay so what you can see here is that At this particular point, okay, if you take the, okay, let us start with the blue lines, okay. So, the blue lines that you see over here are basically the bands of this particular lattice, right. And there are some dust lines also seen which are basically in grey, okay.

So, this dust lines are representing the light lines, okay. okay. That means if you do not have this thing and you just have you know a homogeneous lattice how it will look like. Now at gamma equals gamma beta equals 0 okay that is here which means you know it is basically very very long. lambda with respect to lattice okay so at this particular point you know the wavelength will be able to see the periodic crystal as a average material and that is why you can see that here the blue line and the desk line are more or less you know overlapping but as you move away from this point gamma okay So you are actually having wavelengths which are now getting comparable to the lattice and the wave will start interacting with the lattice and that is why you will see the deviation of these dashed lines okay from the blue lines and this is what is called dispersion. So this is something also very important that we can see from the band diagram.

Now if you consider the slope of a line connecting a point on a band to the gamma point. So if you take the slope of that line you can find out what is the phase velocity okay. So Vp is omega by beta okay and normal at that point on the band Okay if you take a normal of at that particular point on the band okay that will give you the group velocity which is basically derivative in the k space okay. So it is basically d dou omega by dou beta right. So, this also tells you you know the speed at which

the power flows.

And here you can see that there are some you know this region there is a wider gap ok. But here the overall gap for all the direction is only this gray region. So this is the band gap. So the band gap has to be for all the directions. Here also you can see that the gap here, the yellow region here, marks a wider gap between only in this region.

But overall in this particular case, the gray region marks the band gap. Okay, so if you look into the transmittance spectrum, okay, so this is 0 and this is 1. So this is the highest transmission. So what happens when you hit this particular band gap, your transmission is basically dropping to 0. and then you recover and go to high transmission okay and wherever you are hitting the band gap your transmission drops to 0.

So, there can be multiple bands band gap at higher frequencies in a particular crystal right. So, this is all about the lecture on photonic band structure computation and analysis. I hope you understood how band diagrams are obtained and how a normal band diagram can gives you the information of the complete band diagram the 3D one that you have seen okay




So, if you have got any queries regarding this lecture you can write an email to me mentioning MOOC and photonic crystal on the subject line. Thank you.