Course Name- Nanophotonics, Plasmonics and Metamaterials

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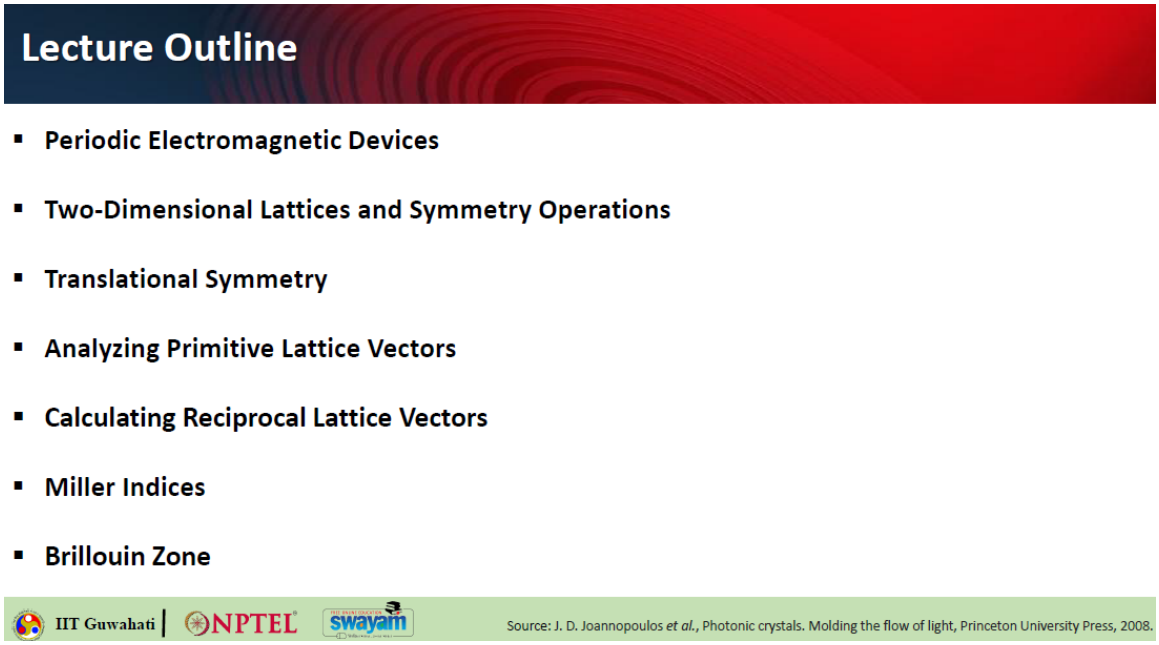
Week-05

Lecture -13

Hello students, welcome to lecture 13 of the online course on Nanophotonics, Plasmonics and Metamaterials. Today we will be covering real and reciprocal lattices.So here is the lecture outline. So today we will have a look at the periodic electromagnetic devices like why we are studying these topics and where is the final objective. We will also go into the technical details like two-dimensional lattices, study about their symmetry operations. We will also understand the translational symmetry that is present in this periodic devices.

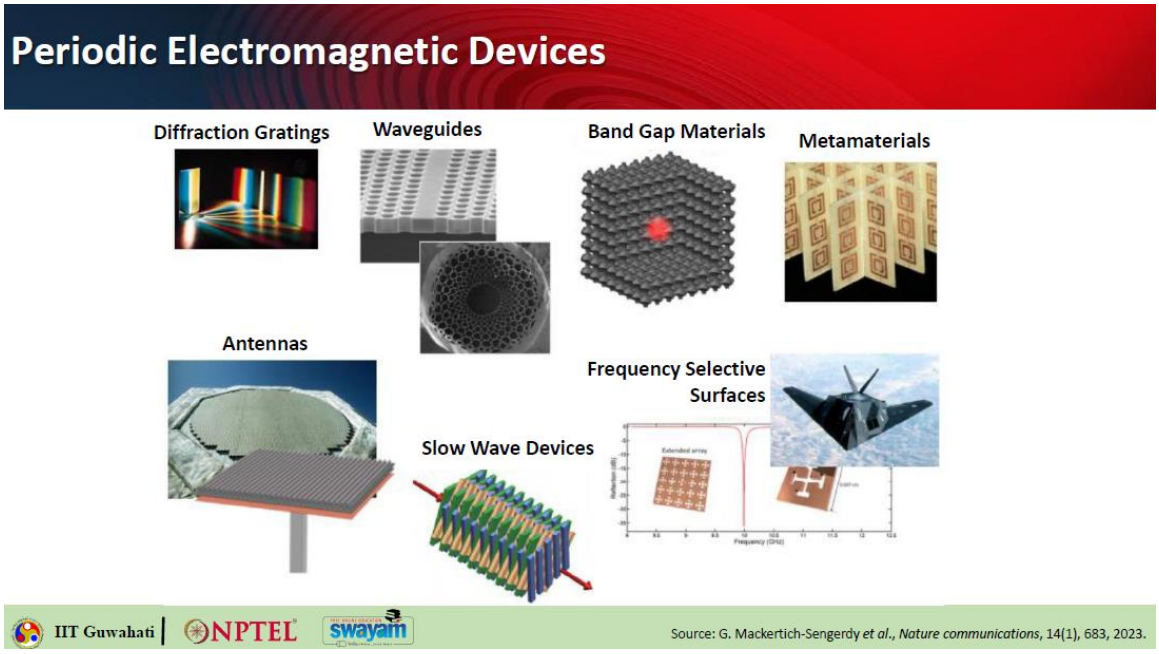


We will analyze the primitive lattice vectors, calculate the reciprocal lattice vectors, obtain Miller indices and also discuss about the Brillouin zones. So here is the final objective. So as you can see we actually use a lot of periodic electromagnetic devices in our different applications. Starting from diffraction grating, you might have heard of this diffraction gratings that allow you to split light into different colors.

So you can use it for spectral imaging. You can use photonic crystals as waveguides for guiding light. You can also have photonic crystal based fibers, hollow core fibers, okay.

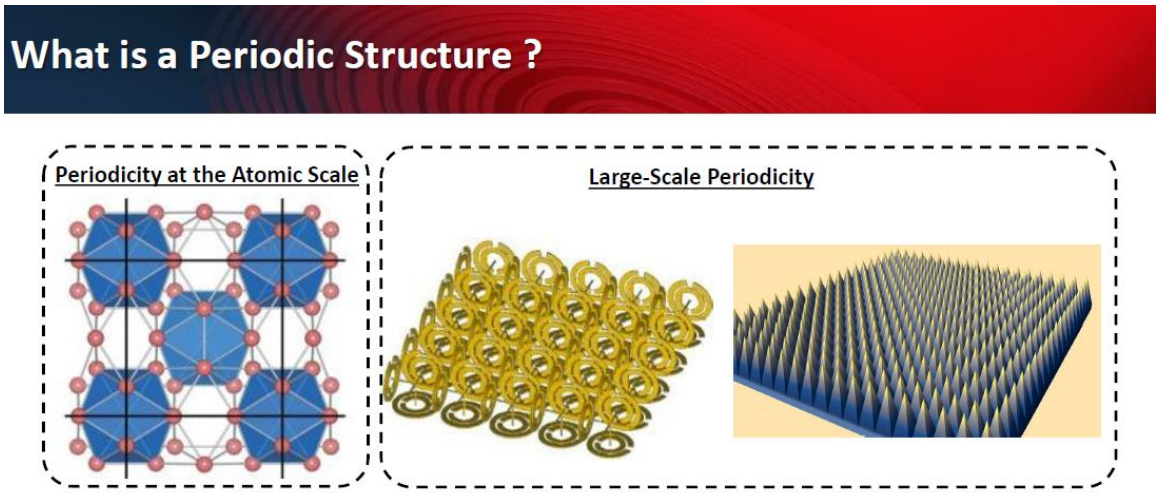
Then you can actually make band gap materials with a defect at the center which will allow you to act, this will act as a resonator cavity. These periodic structures can also form metamaterials as we have discussed initially that you can actually engineer the electromagnetic properties of material using this kind of periodic arrangements.

Obviously you can make antennas, okay, and slow wave devices. You can also make frequency selective surfaces that are also useful for say stealth application. So you can understand that starting from you know optical branches to data communication on chip, data communication over cables, resonator cavity, metamaterials, antennas, frequency selective surfaces, all this application have in a, they use periodic electromagnetic structures. So that is why it is very important to understand these structures in little bit of details and that is the reason why we are discussing this photonic crystal that is the first example of the periodic devices we are dealing in this course in little bit of depth. So let us first go and ask the question that what is a periodic structure? So, if you look into periodicity that is present at the atomic scale.



So all these atoms they actually have a periodic lattice in which the electrons or the elements are oriented or their positions. So different atoms they are all positioned in different lattice points. And if you copy that natural thing into your engineered object you can also make periodic arrangement of different structures which are periodic in two dimension or three dimension depending on your application need Here also, you have largescale periodicity, here we have discussed about So here also atomic scale periodicity. Now because it is periodicity the math describing these things in both this atomic scale and large scale they are basically same. Now how do you describe periodic structures? There is an infinite number of ways that the structures can be periodic.

Just like this we need to find a way to describe and classify periodic lattices. So we have to make generalization to do this. So what are the generalization? So let us see that we can classify periodic structures into 230 space groups which can be classified into 32 crystal groups or you can say they can be classified into 14 Bravais lattices. I believe from the material science kind of courses you might have heard about the 14 Bravais lattices that is present and they also fall under 7 crystal systems. So, these are kind of generalization.



So as you see so this is as you go down they become less specific and they are becoming more generalized. Now what are these space groups? These are set of all possible combinations of symmetry operations that restore the crystal to itself. Okay so what are the different possible combinations of operation you can perform on a particular crystal. Now if you take the example of the 14 Bravais lattice they basically are the primitive lattices. That means these are set of all possible ways a lattice can be periodic if composed of identical spheres placed at the lattice points.

Describing Periodic Structure

- There is an infinite number of ways that structures can be periodic.
- Despite this, we need a away to describe and classify periodic lattices. We have to make generalization to do this.
- We classify periodic structures into:
  - 230 space groups
  - 32 crystal classes
  - 14 Bravais lattices
  - 7 crystal systems

  Less specific
  More generalizations
- Space Groups: Set of all possible combinations of symmetry operations that restore the crystal to itself
- Bravais Lattices: Primitive lattices — set of all possible ways a lattice can be periodic if composed of identical spheres placed at the lattice points.
- Crystal Systems: Set of all Bravais lattices that have the same holohedry *i.e.* shape of the conventional unit cell.

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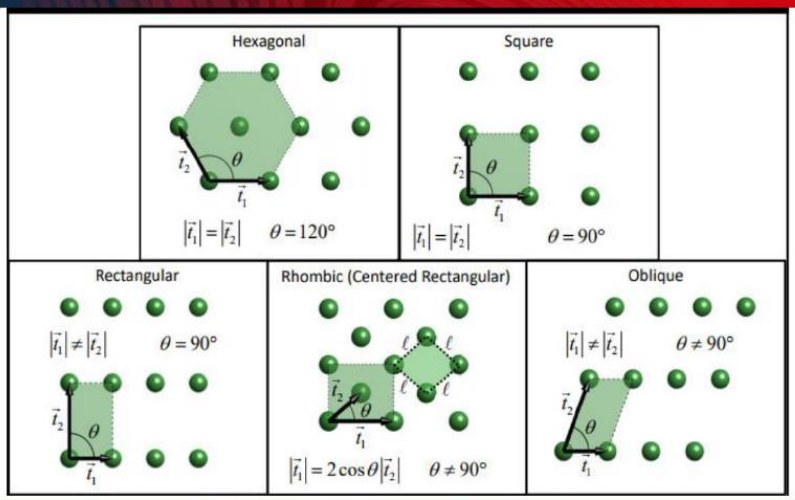
Source: B. Cantor, The Equations of Materials, Oxford University Press, 2020.

So these are like lattices are the structure at which you can repeat the unit cell. So here if you take identical spheres as your unit cell that you can place at every lattice point and that will create that particular arrangement. Okay so when you talk about crystal systems, crystal systems are basically set of all Bravais lattices that have the same holohedry that means the shape of the conventional unit cell. So if you actually look into the classification based on crystal systems there are only 7 crystal systems. So here they are basically the set of all Bravais lattices which have the same shape of the conventional unit cell.

Two-Dimensional Bravais Lattices



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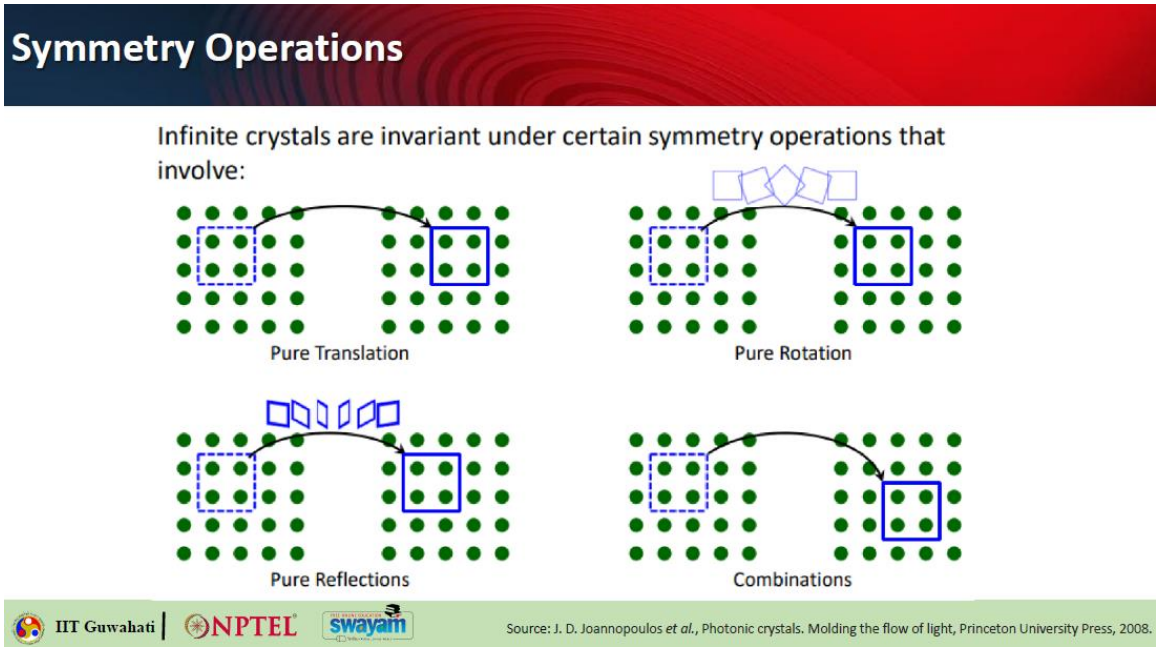
Source: B. Cantor, The Equations of Materials, Oxford University Press, 2020.

Let us look into some of these examples. So if you take 2D Bravais lattices so here you see this is one lattice so you look at the arrangement here this is basically hexagonal. So

you see the green shaded region that shows a hexagonal shape. So at each of this point what is sitting there it is a sphere or an atom or any other shape can actually sit here okay to make this particular lattice. So what are the important things you have to see that here the two lattice vectors they are equal in size and the angle between them is 120 degree.

So that is hexagonal lattice. You can also have square lattice. So here the two lattice vectors are equal in size and the angle between them is 90 degree. Make sense? In rectangular you have to understand that the two lattice vectors are no longer equal okay so this will be longer and this will be shorter but the angle between them has to be 90 degree. There can be other shape like rhombic or centered rectangular like this it is a rectangle with one at the center.

So in that case this is how the two lattice vectors are related and here also the angle requirement is not 90 degree. You can also have oblique like this where modulus of t1 is not equal to t2 that means the two lattice vectors are not equal to each other and their angle is also not 90 degree. These are like two-dimensional previous lattices. When we talk about symmetry operations these are the symmetry operations we discuss. So, one is called pure translation it means moving.



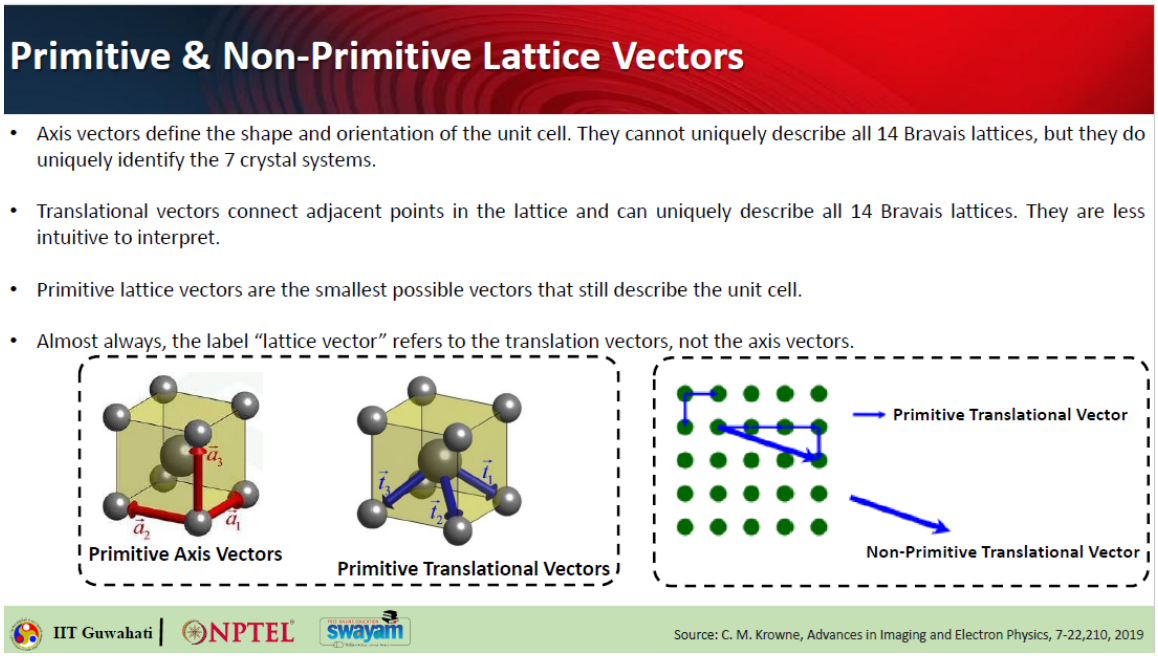
So if you move these to this point okay the lattice orientation remains same. So this is translation symmetry. Then you have rotation symmetry. So if you take this one and rotate it like this okay you see upon this kind of rotation it again gets back to the same shape. So this is called rotation symmetry.

Then you take this one this is called reflection symmetry. So if you take this part and take reflection of it you will see you will get up the same kind of shape. So this is

rotation symmetry and you can also try any combination of this translation, rotation and reflection sorry this is called reflection symmetry. So you can have any combination of translation, rotation and reflection and that combination also give you a identical kind of transformation. So these are called you know symmetry operations.

Now with that let us try to understand the primitive and non-primitive lattice vectors in more details. So as we understood that the axis vector define the shape and the orientation of the unit cell. They cannot uniquely describe all 14 Bravais lattices but they could uniquely describe the 7 crystal system okay. So the translational vectors they connect adjacent points in the lattice and can uniquely describe the 14 Bravais lattices. So these are the two important thing.

One is axis vectors which are good for 7 crystal systems but not good for the Bravais lattices whereas the translational vectors are good for the Bravais lattices okay. Now the primitive lattice vectors are nothing but the smallest possible vectors that can describe the unit cell. We will take this as an example. So if you take this as your unit cell as you can see this is basically a BCC structure body centered cubic structured okay and here you can see that you have taken these are the three vectors. So, you can say these are the primitive axis vectors.



Whereas if you try to take the center point from the center point if you are trying to connect the vectors to the adjacent three points that is the primitive translational vector okay. So these are two different types of orientation or you can say nomenclature or systems. So one is axis vector this way they are defined another is translational vector this is how they are defined. So almost always the level lattice vectors refer to

translational vectors. So when we say lattice vectors we basically mean these vectors which are able to uniquely describe the 14 Bravais lattices.

So always remember like lattice vectors you have to uniquely describe the lattices that is why we go for translational vectors okay. Now this one this is a primitive translational vector this one and this one. How about this? This is also a vector which is you know integral multiple of that particular primitive vector and then you have one along this side. So what about this one? Is this vector a primitive one? No it is not a primitive one okay. The primitive ones are the smallest possible vectors.

So these are the smallest possible vectors not this one okay. So this is the primitive translational vector as you can see here but this one is not the primitive one. So it is a non-primitive translational vector. Now let us look into the translational symmetry. So continuous translational symmetry can be observed okay in such a system where it is unchanged if we translate everything through the same distance in a certain distance certain direction like if you go back here and you see that if you shift the entire system then it is actually the system is unchanged.

So that kind of symmetry is called translation symmetry okay. So given this information we can determine the functional form of the systems modes. Now a system with traditional or translational symmetry is unchanged by a translation through a displacement d. So we are quantifying the thing here. Now for each d we can define a translational vector Td cap okay which on operating on a function f(r) so if you operate this Td cap the translation on a function f(r) it will shift the argument by the distance d and what do we want? We want after the translation it should be same as the original system.

Translational Symmetry

- Continuous translation symmetry — Such a system is unchanged if we translate everything through the same distance in a certain direction. Given this information, we can determine the functional form of the system's modes.
- A system with translational symmetry is unchanged by a translation through a displacement *d*. For each *d*, we can define a translation operator $\hat{T}_d$ which, when operating on a function $\boldsymbol{f(r)}$, shifts the argument by $\boldsymbol{d}$.
- A system with **continuous** translation symmetry in the z direction is invariant under all of the $\hat{T}_d$s for that direction.
- What sort of function is an eigenfunction of all the $\hat{T}_d$s ?
- We can prove that a mode with the functional form e^{ikz} is an eigenfunction of any translation operator in the z direction

$$\hat{T}_{d\hat{z}} e^{ikz} = e^{ik(z-d)} = (e^{-ikd}) e^{ikz} \qquad \text{(L13.1)}$$

- The corresponding **eigenvalue** is $\boldsymbol{e^{-ikd}}$.

IIT Guwahati | NPTEL swayam Source: J. D. Joannopoulos *et al.*, Photonic crystals. Molding the flow of light, Princeton University Press, 2008.

Now a system with continuous translational symmetry in the z direction is basically invariant under all the Tds that can have in the particular direction okay. Continuous translational symmetry means if a system for any value of d is able to repeat itself that is like a continuous translational symmetry system. Now what sort of function is an eigenvalue of all this Tds okay we can prove that a mode with the functional form e to the power ikz is the eigenfunction of any translational operator in z direction. How it works? It works like this. So if you take this translation operator okay at any translation for any distance say d that works on this one so that will actually shift the argument by d.

So how it shifts? $e^{ik(z-d)}$ so that can be written as $\left(e^{-ikd}\right)e^{ikz}$. So this becomes a eigenvalue equation okay and this is the eigenfunction right. This is the eigenvalue this is the eigenfunction okay. So the eigenvalue is e to the power minus ikd. So this is happening for any kind of translation continuous translation.

Now what about we have discrete translational symmetry? It means you cannot repeat at any arbitrary distance but at a defined distance if you repeat the system you will see the same property that is what is called discrete translational symmetry. Now photonic crystals which are man-made crystals okay like traditional crystals of atoms or molecules they do not have continuous translational symmetry. Rather photonic crystals will exhibit discrete translational symmetry that means they are not invariant under translation of any distance but they will work for a given distance and its integral multiple okay. So you can actually take this particular example as you can see that it is a 1D periodic crystal or photonic crystal where it is periodic along the y-axis okay. So what is the period here? It is shown in this box.

Discrete Translational Symmetry

- Photonic crystals, like **traditional crystals of atoms or molecules**, do not have **continuous translational symmetry**. Instead, they have ***discrete* translational symmetry**. That is, they are not invariant under translations of *any* distance, but rather, **only distances that are a multiple of some fixed step length**.

- The simplest example of such a system is a structure that is repetitive in one direction, like the configuration in **Figure.**

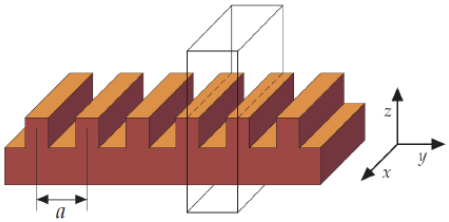


Figure: A dielectric configuration with discrete translational symmetry. If we imagine that the system continues forever in the *y* direction, then shifting the system by an integral multiple of *a* in the *y* direction leaves it unchanged. The repeated unit of this periodic system is framed with a box.

Source: J. D. Joannopoulos *et al.*, Photonic crystals. Molding the flow of light, Princeton University Press, 2008.

So this particular is the unit cell that is being repeated and the repetition is happening at a distance of a okay. So at any sample point at a or integral multiple of a in plus and minus direction you will have the same property. So these are basically systems with discrete translational symmetry right. Now for this system we still have continuous translational symmetry is there but that is along the x. So here it is continuous okay along x direction the system is having continuous translational symmetry but along y direction it is having discrete translational symmetry.

So the basic step length is the lattice constant a and the basic step vector is called the primitive lattice vector. In this case what is the primitive lattice vector? It will be bold a that is nothing but a y cap. It means it is the it is along the y direction and the magnitude is a, okay. That is how you can actually define the primitive lattice vector. Now why only one vector because this is 1D periodic.

You are not bothered about what is happening in the other two dimensions. So periodicity is only seen in y. Now for the system yeah so in this case what you can write that along y it is periodic along x it is also it is having continuous translational symmetry along y it is having discrete translational symmetry. What is happening along z axis? Along z axis you will see that the permittivity is a function of the distance because it is changing with the coordinate z. So here it is say the material is there when you go up you may have the material or may not have the material.

Analyzing Primitive Lattice Vector

- For this system we still have continuous translational symmetry in the x direction, but now we have discrete translational symmetry in the y direction.
- The basic step length is the **lattice constant** a, and the basic step vector is called the **primitive lattice vector**, which in this case is $\mathbf{a} = a\hat{y}$.

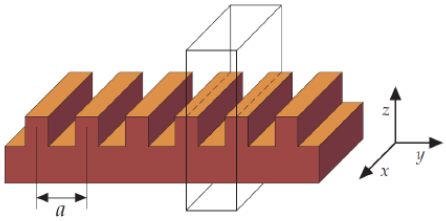


Figure: A dielectric configuration with discrete translational symmetry. If we imagine that the system continues forever in the y direction, then shifting the system by an integral multiple of a in the y direction leaves it unchanged. The repeated unit of this periodic system is framed with a box.

So it is basically changing okay and along y so what is happening the dielectric function you can say it continuously varies in the z direction. So here you will see a continuous variation okay. However along y you will see that it is varying discretely like epsilon r can be written as epsilon r plus minus a. So whatever you are seeing at position r will can also be seen at position r plus a or r minus a. Now by repeating this translation, you can see that epsilon r can be written as epsilon small r plus capital R.

Analyzing Primitive Lattice Vector

- The dielectric function continuously varies in the z direction: $\varepsilon(\mathbf{r}) = \varepsilon(z)$ and discretely in y direction : $\varepsilon(\mathbf{r}) = \varepsilon(\mathbf{r} \pm \boldsymbol{a})$.
- By repeating this translation, we see that $\varepsilon(\mathbf{r}) = \varepsilon(\mathbf{r} + \boldsymbol{R})$ for any $\boldsymbol{R}$ that is an integral multiple of $\boldsymbol{a}$; that is, $\boldsymbol{R} = l\boldsymbol{a}$, where l is an integer.

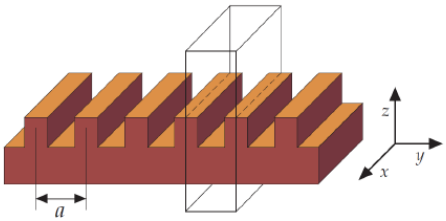


Figure: A dielectric configuration with discrete translational symmetry. If we imagine that the system continues forever in the y direction, then shifting the system by an integral multiple of a in the y direction leaves it unchanged. The repeated unit of this periodic system is framed with a box.

IIT Guwahati | NPTEL swayam Source: J. D. Joannopoulos *et al.*, Photonic crystals. Molding the flow of light, Princeton University Press, 2008.

So what is capital R? It will be nothing but any integral multiple of the lattice period which is small a. So R can be written as l a, l is the integer. These are very simple things okay. Now the dielectric unit that we have considered we considered to be repeated over and over just like this box is being repeated okay. Now what is this box called? In good

terms it is called unit cells okay because this is the thing that is being repeated periodically.

Now in this example the unit cell is an x z slab of dielectric material which has got a width a in the y direction. So if you describe your unit cell like this it is clear that it is a 1D periodic structure. Now because of the translational symmetries eigenfunctions must commute with all of the translation operation in the x direction as well as the translation operators for lattice vectors that is R equals l a y in the y direction. So, with this knowledge we can identify the modes of simultaneous eigenfunctions of both translational operators.

Analyzing Primitive Lattice Vector

- The dielectric unit that we consider to be repeated over and over, highlighted in **Figure** with a box, is known as the **unit cell**. In this example, the unit cell is an xz slab of dielectric material with width a in the y direction.
- Because of the translational symmetries, eigenfuntions must commute with all of the translation operators in the x direction, as well as the translation operators for lattice vectors $R = la\hat{y}$ in the y direction.

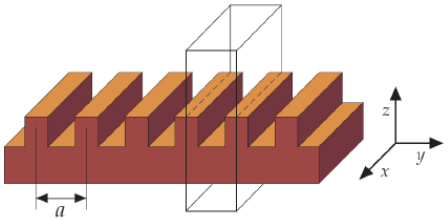


Figure: A dielectric configuration with discrete translational symmetry. If we imagine that the system continues forever in the y direction, then shifting the system by an integral multiple of a in the y direction leaves it unchanged. The repeated unit of this periodic system is framed with a box.

Source: J. D. Joannopoulos *et al.*, Photonic crystals. Molding the flow of light, Princeton University Press, 2008.

So there are two types of operator as I mentioned. So, you have this $\hat{T}_{d\hat{x}}e^{ik_x x}$ that is along x it is a continuous translational symmetry. So, this will be the eigenvalue operation okay and along y you have this discrete translational symmetry and that happens along R that is l a integral multiple of the lattice period. So, these are the two you know translation operation that is happening and using this you can identify the modes of simultaneous eigenfunctions okay. Now let us see how do you calculate the reciprocal lattice vectors. Now we can begin to classify the modes by specifying kx and ky okay.

Analyzing Primitive Lattice Vector

- With this knowledge, we can identify the modes of simultaneous eigenfunctions of both translation operators as:

$$\hat{T}_{d\hat{x}} e^{ik_x x} = e^{ik_x(x-d)} = (e^{-ik_x d}) e^{ik_x x} \quad \text{(L13.2)}$$

$$\hat{T}_{\mathrm{R}} e^{ik_y y} = e^{ik_y(y-\ell a)} = (e^{-ik_y \ell a}) e^{ik_y y} \quad \text{(L13.3)}$$

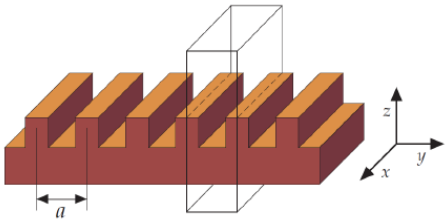


Figure: A dielectric configuration with discrete translational symmetry. If we imagine that the system continues forever in the *y* direction, then shifting the system by an integral multiple of *a* in the *y* direction leaves it unchanged. The repeated unit of this periodic system is framed with a box.

So kx and ky they are in the momentum space right. Now however not all values of ky will yield different eigenvalues. Consider two modes one with wave vector ky and another with wave vector $k_y + 2\pi / a$ okay. Now what is this 2 pi by a? a is the lattice constant. So you can have wave vector with these two values. Now if you insert these values into the equations that you have seen here these two equations okay they will show that they have the same Tr cap eigenvalues okay.

Calculating Reciprocal Lattice Vectors

- We can begin to classify the modes by specifying k_x and k_y. However, not all values of k_y yield different eigenvalues. Consider two modes, one with wave vector k_y and the other with wave vector $k_y + 2\pi/a$.
- A quick insertion into (L13.2 & L13.3) shows that they have the same $\hat{T}_R$ eigenvalues. In fact, all of the modes with wave vectors of the form $k_y + m(2\pi/a)$, where m is an integer, form a degenerate set; they all have the same $\hat{T}_R$ eigenvalue of $e^{-i(k_y l a)}$.
- Augmenting k_y by an integral multiple of $b = 2\pi/a$ leaves the state unchanged. We call $b = b\hat{y}$ the primitive **reciprocal lattice vector**.
- Suppose we have a function *f* (**r**) that is periodic on a lattice; that is, suppose *f* (**r**) = *f* (**r** + **R**) for all vectors **R** that translate the lattice into itself (i.e., connect one lattice point to the next). Our dielectric function $\varepsilon(\mathbf{r})$ is an example of such a function. The vectors **R** are called the **lattice vectors**.

In fact all of the modes with the wave vectors of the form $k_y + m(2\pi / a)$,m is an integer they will form a degenerate set and they all will have the same Tr cap eigenvalue of e to the power minus i ky l a okay. So it means all these cases they will actually have the

same eigenvalues. Now this was done for say ky right. So augmenting ky by an integral multiple of b so if you define 2 pi by a as b okay so this is nothing but integral multiple of b okay. So, you understand that this will leave the state unchanged.

So you can actually call b equals by cap as the primitive reciprocal lattice vector right. So real lattice and reciprocal lattice, reciprocal lattice is in the momentum space and there you can understand that whatever is you are adding integral multiple of that thing that repeats so that will give you the reciprocal lattice vector. Now suppose we have a function f r that is periodic on a lattice. So periodic means you can write that f of r will be same as f of small r plus capital R for all the vectors capital R that translate the lattice into itself. So, it is repeating after this particular value of capital R.

So we have seen what is capital R that is basically small l a, l is integer a is the lattice constant right. Now our dielectric function epsilon r can also be taken as this kind of function. So instead of f, f was a generic one you can think of a property material property like permittivity that will also repeat using this particular relationship. And in this case capital r is called the lattice vector okay. Now if you consider a two dimensional arrangement, so let us consider this particular picture which is a periodic structure of identical parallel rods or tubes or vanes, vanes will be like meshes okay like grids like this okay.

Calculating Reciprocal Lattice Vectors

- Consider a periodic structure such as a set of identical parallel rods, tubes, or veins embedded in a homogeneous host medium and organized at the points of a rectangular lattice, as illustrated In **Figure.**

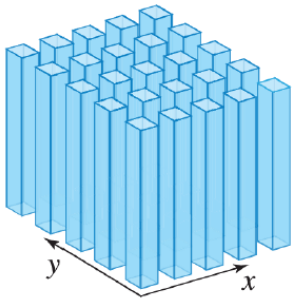


Figure: Rectangular Lattice.

- The impermeability $\eta(x,y) = \epsilon o/\epsilon(x,y)$ is periodic in the transverse directions, x and y, and uniform in the axial direction z. If a_1 and a_2 are the periods in the x and y directions, then $\eta(x,y)$ satisfies the translational symmetry relation

$$\eta(x + m_1 a_1, y + m_2 a_2) = \eta(x,y) \qquad \text{(L13.4)}$$

for all integers m_1 and m_2. This periodic function is represented as a two-dimensional Fourier series,

$$\eta(x,y) = \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell_2=-\infty}^{\infty} \eta_{\ell_1,\ell_2} \exp(-j\ell_1 \boldsymbol{g}_1 x) \exp(-j\ell_2 \boldsymbol{g}_2 x) \qquad \text{(L13.5)}$$

Source: B. E. Saleh and M. C. Teich, Fundamentals of photonics, John Wiley & Sons, 2019.

So you can assume these vanes to be embedded in a homogeneous host medium and they are organized at the points of a rectangular lattice. So what is happening here you can think of a you know square or rectangular lattice. So rectangular lattice as I mentioned before that one lattice vector is not equal to the other lattice vector that is rectangular lattice but you have to make sure the angle is 90 degree. In this case the

impermeability which is $\eta(x,y) = \epsilon_0 / \epsilon(x,y)$. Now this is also periodic in the transverse directions that is x and y however it is uniform along the z direction because there is no change in the z direction it can be infinitely large in the z direction okay.

Now if a1 and a2 are the periods in the x and y direction so if you consider the period here is a1 and this is a2 so the shortest distance here will be a1 and a2 so they are the lattice vectors right. So you can say that eta xy satisfies the translational symmetry relation given by this. So, what is that $\eta\left(x + m_1 a_1, y + m_2 a_2\right) = \eta(x,y)$. So that is how you can also understand that for all integer values of m1 and m2 this relation will be satisfied.

So this is a periodic 2D lattice. This periodic function is represented as a two-dimensional Fourier series in the form of this one. So any periodic function can be expressed as a Fourier series that you have learnt. So eta xy can be written as all these different components here okay. You can write $\eta(x,y) = \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell_2=-\infty}^{\infty} \eta_{\ell_1,\ell_2} \exp\left(-j\ell_1 g_1 x\right) \exp\left(-j\ell_2 g_2 x\right)$.

Now what are this g1 and g2 we have seen in the previous lecture. $g_1 = 2\pi / a_1$ and $g_2 = 2\pi / a_2$ these are the fundamental spatial frequency along x and y direction. What will be the unit radian per mm okay and l1 g1 and l2 g2 are nothing but they are harmonics because any frequencies spatial frequencies fundamental frequency if you multiply them within integers you will get their harmonics right. So the coefficients that you have seen eta l1 l2 depend on the actual profile of the periodic function that is the size or the shape of the rods. So, let us look into the 2D Fourier transform of the period function.

Calculating Reciprocal Lattice Vectors

- $g_1 = 2\pi/a_1$ and $g_2 = 2\pi/a_2$ are fundamental spatial frequencies (radians/mm) in the x and y directions, and $l_1 g_1$ and $l_2 g_2$ are their harmonics. The coefficients $\eta_{l_1 l_2}$ depend on the actual profile of the periodic function, *e.g.*, the size of the rods.

- The two-dimensional Fourier transform of the periodic function is composed of points on a rectilinear lattice, as shown in **Figure (b)**. This Fourier-domain lattice is known to solid-state physicists as the **reciprocal lattice**.

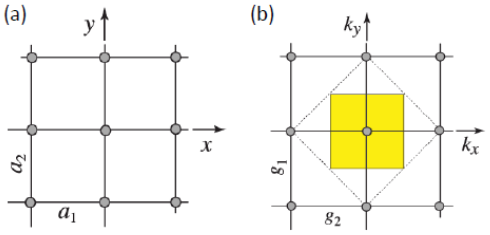


Figure: (a) The rectangular lattice at which the rods are placed. (*b*) The two-dimensional Fourier transform of the lattice points is another set of points forming a reciprocal lattice with periods $g_1 = 2\pi/a_1$ and $g_2 = 2\pi/a_2$.

Source: B. E. Saleh and M. C. Teich, Fundamentals of photonics, John Wiley & Sons, 2019.

So it is composed of points on a rectilinear lattice as shown in B. So this is the real lattice which is basically the lattice points are shown here okay. So we have considered a rectangular lattice so this lattice vector is a1 this is a2 but when you convert it into the reciprocal lattice that is in the Fourier domain okay you went to the from space you have gone to momentum space okay. So here you will call it kx and ky okay and this lattice vectors are now 2 pi by a1 so it is g1 okay and g2 okay they can be yeah $g_1 = 2\pi / a_1$ and $g_2 = 2\pi / a_2$. I think there is a typo here okay that can be corrected. So this should have been g1 and this is g2 so this is how you get the reciprocal lattice fine. Now once you understood that how you get the reciprocal lattice what are the optical modes of the medium with such symmetry that you have to find out okay and there will be another important thing that what is this particular region that we have marked here okay.

Calculating Reciprocal Lattice Vectors

- What are the optical modes of a medium with such symmetry?
- For waves traveling in a direction parallel to the *x*–*y* plane, the modes are two-dimensional Bloch waves:

$$U(x,y) = p_{K_x,K_y}(x,y)\exp(-jK_x x)\exp(-jK_y y) \quad \text{(L13.6)}$$

where p_{K_x}, $p_{K_y}(x,y)$ is a periodic function with the same periods as the medium

- The wave is specified by a pair of Bloch wavenumbers (K_x, K_y). Another wave with Bloch wavenumbers ($K_x + g_1$, $K_x + g_2$) is not a new mode. As shown in **Figure**, a complete set of modes in the Fourier plane has Bloch wavenumbers located at points in a rectangle (in yellow) defined by $[-g_1/2 < K_x \le g_1/2]$ and $[-g_2/2 < K_y \le g_2/2]$, which is the first **Brillouin zone**.

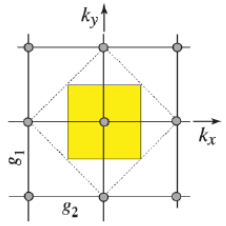


Figure: Reciprocal Lattice (The shaded (yellow) area is the Brillouin zone).

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Source: B. E. Saleh and M. C. Teich, Fundamentals of photonics, John Wiley & Sons, 2019.

Now if you consider the waves traveling in the direction parallel to the xy plane the modes of the two-dimensional block waves are given by $U(x,y) = p_{K_x,K_y}(x,y)\exp(-jK_x x)\exp(-jK_y y)$, where this is basically the periodic function with the same period as the medium. Now if you consider this particular reciprocal lattice the shaded region the yellow shaded region here is basically the Brillouin zone. So how do you get Brillouin zone we will come to that but first of all you have to remember that the wave that is shown here is basically having a pair of block wave numbers it has got kx and ky right. So another wave with block wave numbers like kx plus g1 and ky plus g2 okay that will not be a new mode rather they will kind of they will be same. As shown in the figure a complete set of modes in the Fourier plane has block wave numbers located at points in the rectangle defined by this one.

So what is this one? So kx is defined as minus g1 by 2 to g1 by plus g1 by 2 and ky will be defined as minus g2 so this is 2 okay minus g2 by 2 to plus g2 by 2 and this particular rectangle is called the first Brillouin zone. And why we are interested here so if you are able to calculate all the modes in this particular zone we know it for the entire lattice. So other symmetries may be used to reduce the set of independent block mode wave vectors within the Brillouin zone. So we will come to that concept which is also known as how to find out the irreducible Brillouin zone. So, when all the symmetries are included the result in an area called irreducible the result is an area called irreducible Brillouin zone okay.

Calculating Reciprocal Lattice Vectors

- Other symmetries may be used to reduce the set of independent Bloch wave vectors within the Brillouin zone.
- When all symmetries are included, the result is an area called the **irreducible Brillouin zone**. For example, the rotational symmetry inherent in the square lattice results in an irreducible Brillouin zone in the form of a triangle, as shown in **Figure**.

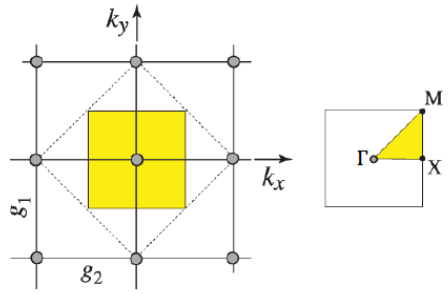


Figure: Reciprocal Lattice. For a square lattice ($a_1 = a_2 = a_3$), the irreducible Brillouin zone is the triangle ΓMX.

Source: B. E. Saleh and M. C. Teich, Fundamentals of photonics, John Wiley & Sons, 2019.

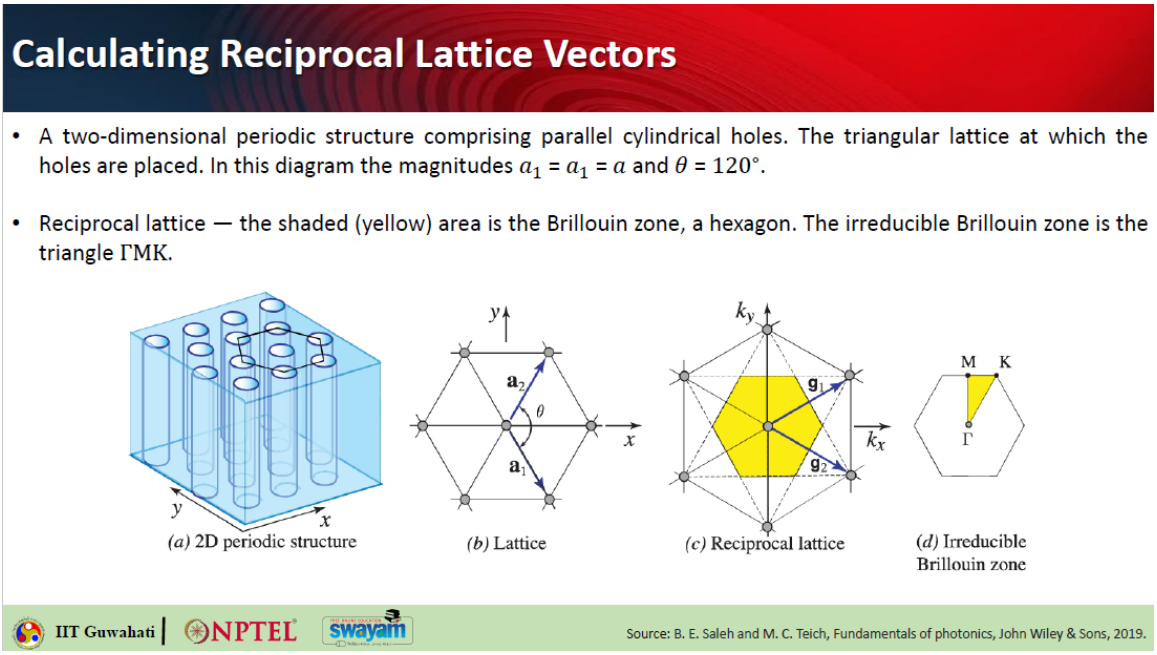
So, we will take an example here that in this particular case you can understand that this is basically a square okay kind of shape. So, here what you can have you know you can actually look for rotational symmetry okay and mirror symmetry. So, from that you can identify that this rectangle sorry this square or rectangle is better is a generic term because g1 and g2 are not same. So, let us take say this rectangle if you take a mirror you get this one and then you put a mirror here the whole thing is formed right.

So, this is the basic Brillouin zone okay. You can start with it and create the whole thing. However taking only half of it because it is also having a rotational symmetry. So, if you take half of it and rotate it by 45 degree you will get the other half okay. So, that way this becomes the irreducible Brillouin zone and there are ways of marking it.

So, you can actually mark this as gamma M X. So, what is M? M is the corner point, X is the midpoint of the edge right. Now a two-dimensional periodic structure comprising parallel cylindrical holes are considered here. So, here one important thing as you can see they are not actually aligned in a rectangular or square lattice. So if you connect all the center points of this cylindrical holes. So, how do you make these holes first of all? You take this structure and then drill holes in this particular pattern.

So, if you mark all the center points of this particular holes you will see this is the lattice okay. So and from this lattice this is the direct lattice. So you can see this is a1, this is a2 both are equal and this angle is around 120 degree. So this is a hexagonal lattice right and or you can also call this as triangular lattice there is another name for it okay. So, from this you can always convert it to the reciprocal lattice space and find out what is g1 and g2 okay and in this reciprocal lattice space you can identify the Brillouin

zone.



How do you do the Brillouin zone? Once again you take the one center point and then you connect it to all other points like this okay. So, you can draw these lines and then you draw perpendicular bisector like this. So, you will get this particular one. For this one you draw another perpendicular bisector you get this one.

For this you draw another perpendicular bisector you get this one. Then you get this one for this line, for this one you get this line, for this one you get this line and that is it. And then you paint this area with yellow and you can just show that this is your reciprocal lattice having this Brillouin zone okay. So, this is the first Brillouin zone okay and from this you can also identify as I mentioned you can use those rotational symmetry and mirror symmetry and all these things. So, you can identify what is the irreducible Brillouin zone. Here you will see that you can identify only this triangle to carry all the information about the Brillouin zone okay.

So that is how irreducible Brillouin zone helps you to reduce the computation and but still give you the same amount of information of a Brillouin zone okay. So this we have already covered so this is in the shape of a hexagon right. Now I think we have already discussed this for a given lattice with a set of lattice vectors R how can we determine all the reciprocal lattice vectors G. So here we are naming the real lattice vectors as capital R and the reciprocal lattice vectors as capital G and let us find out you know that what is the relationship between this G and R okay. So we need to find all G such that if you do G dot R means if you multiply this okay this is some integer multiple of 2 pi for every value of R okay.

So how do you do that? We know that every lattice vector R can be written in terms of its primitive lattice vector which are basically primitive lattice vectors are nothing but the shortest vectors pointing from one lattice point to another lattice point okay. So for example if you take a simple cubic lattice with spacing say small a the vectors capital R can be written in the form of la x plus ma y plus na z. So as you can see it is a cubic lattice so all the distances are basically same a and l, m, n these are basically integer. Now in general we call the primitive lattice vectors there are names a1, a2 and a3 right and they need not be of unit length that is understood only in certain cases they will be equal to each other okay or two may be equal one will be different and so on. And we have already mentioned that the reciprocal lattice vectors which are denoted by G form a lattice of their own okay.

Constructing Reciprocal Lattice Vectors

- Given a lattice with a set of lattice vectors $\boldsymbol{R}$, how can we determine all of the reciprocal lattice vectors $\boldsymbol{G}$? We need to find all $\boldsymbol{G}$ such that $\boldsymbol{G}.\boldsymbol{R}$ is some integer multiple of 2π for every $\boldsymbol{R}$.
- We know that every lattice vector $\boldsymbol{R}$ can be written in terms of the **primitive lattice vectors**, which are the smallest vectors pointing from one lattice point to another. For example, on a simple cubic lattice with spacing a, the vectors $\boldsymbol{R}$ would all be of the form $\boldsymbol{R} = la\hat{x} + ma\hat{y} + na\hat{z}$, where (l, m, n) are integers. In general, we call the primitive lattice vectors a_1, a_2, and a_3. They need not be of unit length.
- We have already mentioned that the reciprocal lattice vectors $\{\boldsymbol{G}\}$ form a lattice of their own. In fact, the reciprocal lattice has a set of primitive vectors b_i as well, so that every reciprocal lattice vector $\boldsymbol{G}$ can be written as $\boldsymbol{G} = lb_1 + mb_2 + nb_3$.
- Our requirement that $\boldsymbol{G} \cdot \boldsymbol{R} = 2\pi N$ boils down to the primitive requirement

$$\mathbf{G} \cdot \mathbf{R} = (\ell \mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3) \cdot (\ell' \mathbf{b}_1 + m'\mathbf{b}_2 + n'\mathbf{b}_3) = 2\pi N \qquad \text{(L13.7)}$$

IIT Guwahati | NPTEL swayam Source: J. D. Joannopoulos *et al.*, Photonic crystals. Molding the flow of light, Princeton University Press, 2008.

So it is a there is a real lattice and there is a reciprocal lattice. In fact the reciprocal lattice has a set of primitive vectors bi so there it is ai or you can say a1, a2, a3 here it will be b1, b2, b3. It means every reciprocal lattice vector G can also be written as $\boldsymbol{G} = lb_1 + mb_2 + nb_3$ and so on where l, m, n are basically integers right. So, our requirement that $\boldsymbol{G} \cdot \boldsymbol{R} = 2\pi N$ boils down to the requirement that this particular product that you have seen okay just to not to confuse that this l, m, n should be equal you can actually mark them as l prime, m prime, and n prime okay that this integer values are basically different to this integer values. But this multiplication should give you 2 pi N. Now for all the choices of l, m, n that you have seen okay there should be some value of N that holds that equation correct.

So if you put some thought you will see that only in the case when $a_i \cdot b_j = 2\pi$ this will happen if i and j are equal and if they are unequal okay this will be unequal there is a typo here you get 0 okay. It means compactly you can write that ai dot bj the two unit

vectors when you multiply them if they are in the same direction you get this value 1 okay if they are in different direction you get 0. So $a_i \cdot b_j = 2\pi\delta_{ij}$ okay this is how you can write it compactly. Now given the set a1, a2 and a3 our task is to then find out the corresponding set of the reciprocal lattice vectors that is b1, b2 and b3 and what is the condition? The condition boils down to ai dot bj should be equal to 2 pi delta ij.

Constructing Reciprocal Lattice Vectors

- For all choices of (l, m, n), the above must hold for some N. A little thought will suggest that we could satisfy the above if we construct the b_i so that $a_i . b_j = 2\pi$ if $i = j$, and 0 if $i = j$.
- More compactly, we write $a_i . b_j = 2\pi\delta_{ij}$. Given the set $\{a_1, a_2, a_3\}$, our task is to find the corresponding set $\{b_1, b_2, b_3\}$ such that $a_i . b_j = 2\pi\delta_{ij}$.
- One way to do this is to exploit a feature of the cross product. Remembering that $x.(x \times y) = 0$ for any vectors x and y, we can construct the primitive reciprocal lattice vectors with the following recipe:

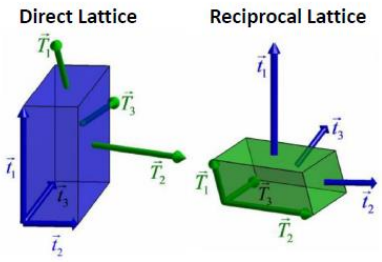
$$\mathbf{b}_1 = \frac{2\pi\,\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad \mathbf{b}_2 = \frac{2\pi\,\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad \mathbf{b}_3 = \frac{2\pi\,\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}. \qquad \text{(L13.8)}$$

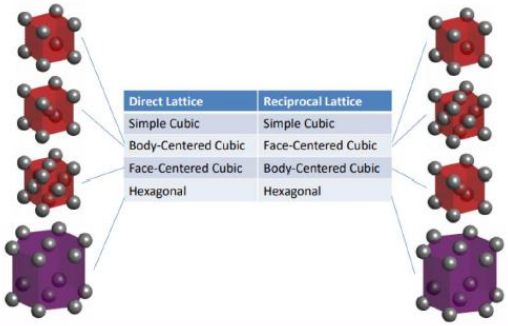
Source: J. D. Joannopoulos *et al.*, Photonic crystals. Molding the flow of light, Princeton University Press, 2008.

Now one way to do this is to exploit a feature of the cross product. So you remember this formula that x dot x cross y equals 0 and that is happening for any vector basically. So if you take x, y as any vectors if you do this particular operation you will get 0. So using that you can also find out that in the primitive reciprocal lattice vectors can be obtained from the real lattice vectors using this formula. So b1, b2, b3 can be obtained from a1, a2 and a3 using this particular relationships okay. In summary we can say that when we take the Fourier transform of a function that is periodic on lattice we need only include the terms with wave vectors that are reciprocal lattice vectors.

Constructing Reciprocal Lattice Vectors

- In summary, when we take the Fourier transform of a function that is periodic on a lattice, we need only include terms with wave vectors that are reciprocal lattice vectors. To construct the reciprocal lattice vectors, we take the primitive lattice vectors and perform the operations of equation (L13.8).
- Each direct lattice has a unique reciprocal lattice so knowledge of one implies knowledge of the other.



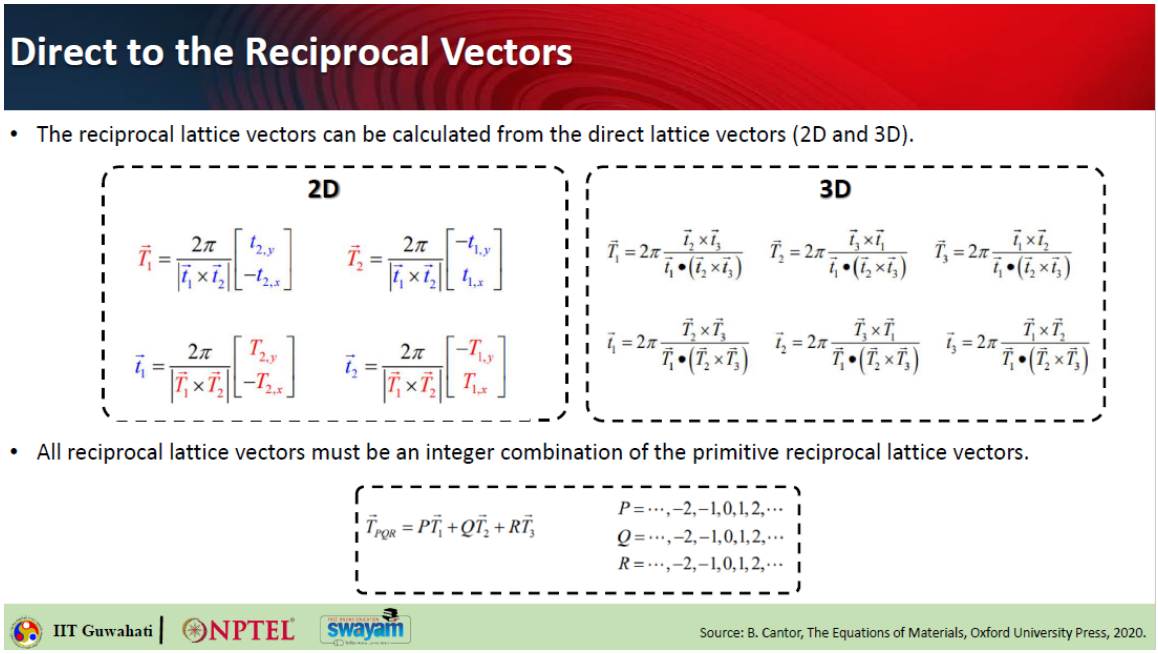


Direct Lattice	Reciprocal Lattice
Simple Cubic	Simple Cubic
Body-Centered Cubic	Face-Centered Cubic
Face-Centered Cubic	Body-Centered Cubic
Hexagonal	Hexagonal

Source: J. D. Joannopoulos *et al.*, Photonic crystals. Molding the flow of light, Princeton University Press, 2008.
Source: C. M. Krowne, Advances in Imaging and Electron Physics, 7-22,210, 2019.

Now to construct the reciprocal lattice vectors we take the primitive lattice vectors and perform the operations that are given in this equation simple. Now each direct lattice has a unique reciprocal lattice. So if you have knowledge of one you have the knowledge of another because they will correspond to uniquely to each other. So if you take a direct lattice like this so the blue one shows the primitive lattice vectors here and in the green one the capital ones are showing the primitive reciprocal lattice vectors.

So you can actually correlate this. So if the direct lattice is simple cubic your reciprocal lattice also turns out to be simple cubic. If you have BCC when you do the reciprocal lattice you will come up with FCC. If you have FCC you will come up with BCC and if you have hexagonal you still come up with hexagonal. So this is how you know they correspond to each other. And this is how you can convert as I have already shown how to convert the reciprocal lattice vectors okay.



So capital t1 and capital t2 are basically the reciprocal lattice vectors okay and the blue ones are basically the small t1 and small t2 are the real lattice vectors. So this is how you can actually now get the values of each other. So these are the values of how to obtain capital t1, capital t2, capital t3 this is for 3D system okay and these are for 2D system. And all the reciprocal lattice vectors must be an integral or integer combination of the primitive reciprocal lattice vector. That means this T_{PQR} or it can be called as G capital g as you have seen they will be nothing but capital p or l prime as you have seen before capital t1 that is the real sorry this is the primitive reciprocal lattice vector T1, T2 and T3 so they are basically integers P,Q,R all these are integers.

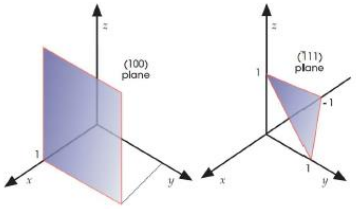
Different books use different notation just remember these concepts okay. And the next important thing is to how to define the different planes using mirror indices. Now miller indices identify repeating planes within the periodic structures like crystals. So if you look into the definition of reciprocal lattice vector this is how we have defined just now. So, P, Q and R they can be called as the mirror indices of the planes in the direct lattice which is described by a reciprocal lattice vector PQR.

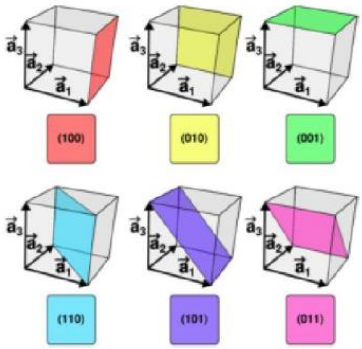
Miller indices

- Miller indices identify repeating planes within the periodic structures like crystals.
- Recall the definition of a reciprocal vector:

$$\vec{T}_{PQR} = P\vec{T}_1 + Q\vec{T}_2 + R\vec{T}_3 \qquad P = \cdots, -2, -1, 0, 1, 2, \cdots \quad Q = \cdots, -2, -1, 0, 1, 2, \cdots \quad R = \cdots, -2, -1, 0, 1, 2, \cdots$$

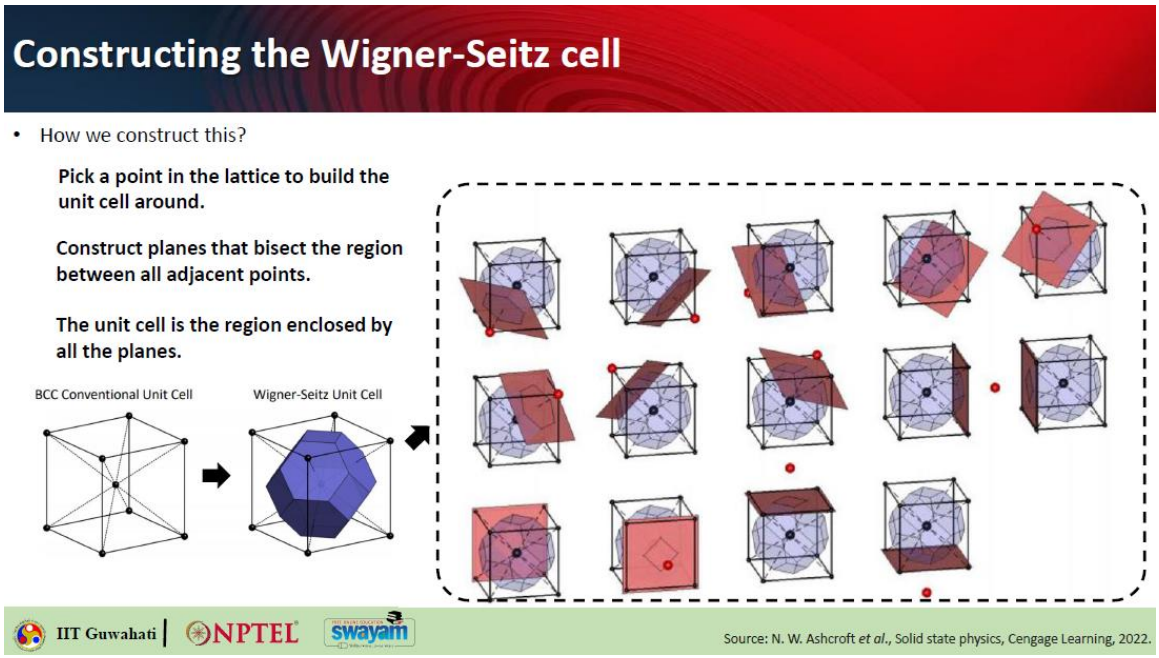
- P, Q, and R are the Miller indices of the planes in direct lattice described by the reciprocal lattice vector $\vec{T}_{PQR}\langle PQR\rangle$.





Source: J. D. Joannopoulos *et al.*, Photonic crystals. Molding the flow of light, Princeton University Press, 2008.
Source: N. W. Ashcroft *et al.*, Solid state physics, Cengage Learning, 2022.

So let us see how it works. So if you have a 1 0 0 plane that means along x you have 1 and it does 0 0 means it will be parallel to both y and c. 1 1 1 plane means it will cut all three axis at oh there is a 1 bar so 1 bar is minus 1 along x okay and then you have 1 along y and 1 along z so this is a particular plane that is given as this mirror indices 1 bar 1 1 okay. You can also have some more like this is if you try to write them in terms of the lattice vectors okay a 1 a 2 and a 3 you can define them as 1 0 0 this one is this yellow region one is 0 1 0 this one is 0 0 1 this is 1 1 and then 0 and so on. So this is how Miller indices help you identify repeating planes within periodic structures. Now the last thing that remains here is to see how do you construct Wigner Seitz cell or the Brillouin zone okay.



We will come to Brillouin zone because the concept that we will see here in Wigner Seitz cell Wigner Seitz cell happens in real lattices and Brillouin zone happens in reciprocal lattices but the concept is very similar okay and the construction of this cell is also very similar. So how do you construct it let us see so pick a point in the lattice to build the cell around so let us pick this particular point okay and then for this point construct planes that bisect the region between all adjacent points okay. So from this point to this point this is the connecting line so you actually put a plane that bisects that region similarly for this to this you put another plane that bisects this region and so on. So when you add up all this you will get this kind of a region unit cell region that is enclosed by all these planes okay. So this is how the construction is done as you can see so from the center point to this point if you take midway you first take that connecting line midway you draw a plane so you basically get this kind of a section here then you have this plane this plane when all these planes add up they will give you this particular shape okay.

Brillouin Zone

- The Brillouin zone is constructed in the same manner as the Wigner-Seitz unit cell, but it is constructed from the reciprocal lattice.
- The Brillouin zone is closely related to wave vectors and diffraction so analysis of periodic structures is often performed in "reciprocal space."
- The Brillouin zone for a face-centered cubic (fcc) lattice is a "truncated" octahedron with 14 slides.
- This is the most "spherical" of all the Brillouin zones so the FCC lattice is said to have the highest symmetry of the Bravais lattice.

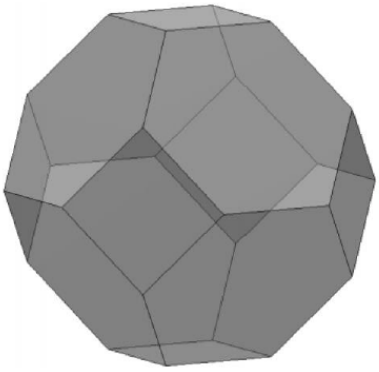


Figure: The Brillouin zone for the face-centered cubic (fcc) lattice.

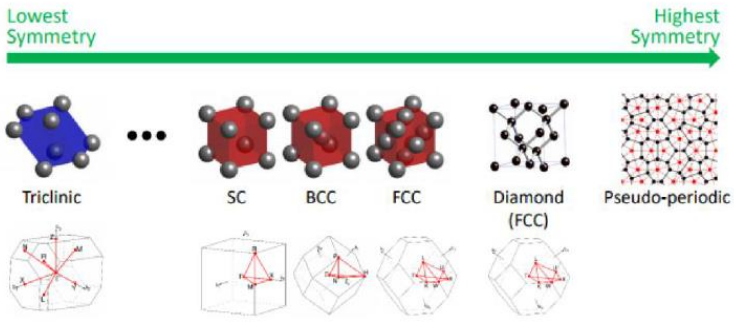
Source: J. D. Joannopoulos *et al.*, Photonic crystals. Molding the flow of light, Princeton University Press, 2008.

So whatever you have done for Wigner Seitz cell if you do the same thing in a reciprocal lattice you will basically get a Brillouin zone okay. So the construction of Brillouin zone is exactly similar as the Wigner Seitz cell just you have to do the same operation in reciprocal lattice. Now Brillouin zone is closely related to wave vectors and diffraction so analysis of periodic structures is often performed in reciprocal lattice. So that is how you know that the study of Brillouin zone becomes very important okay.

The reason is the Brillouin zone is closely related to the wave vectors and diffraction. So if you take the Brillouin zone of a FCC structure that is basically a truncated octahedron like this of 14 sides okay not slides it is 14 sides. So this is basically the most symmetrical Brillouin zone because it is almost spherical. So you can say that FCC lattice is having the highest symmetry among all the Bravais lattice. So, if you try to see the degree of symmetry for different type of crystal and other structures you will see triclinic has got the lowest symmetry whereas diamond which is having FCC structure it has got the highest symmetry okay.

Brillouin Zone

Degree of Symmetry: How spherical the Brillouin zone is.



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Source: N. W. Ashcroft *et al.*, Solid state physics, Cengage Learning, 2022.

And if you go for pseudo periodic like this they have even further increase in symmetry. Now these are the points of symmetry in a Brillouin zone. So this is I am showing this in a 3D crystal. So if you take think of a planar one so if you take a cubic crystal and if you then the important points are gamma, M, R and X. So, these are the points of the irreducible Brillouin zone.

Brillouin Zone: Points of Symmetry

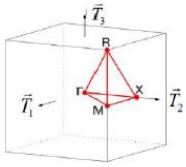
Several points of high symmetry are of special interest – these are called critical points.

Symbol Description

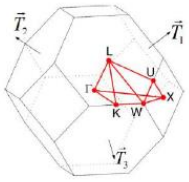
Γ Center of the Brillouin zone

Simple cube

M Center of an edge
R Corner point
X Center of a face



CUB path: Γ-X-M-Γ-R-X|M-R



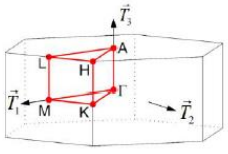
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

Face-centered cubic

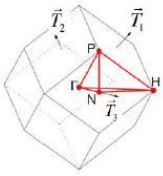
K Middle of an edge joining two hexagonal faces
L Center of a hexagonal face
U Middle of an edge joining a hexagonal and a square face
W Corner point
X Center of a square face

Hexagonal

A Center of a hexagonal face
H Corner point
K Middle of an edge joining two rectangular faces
L Middle of an edge joining a hexagonal and a rectangular face
M Center of a rectangular face



HEX path: Γ-M-K-Γ-A-L-H-A|L-M|K-H



BCC path: Γ-H-N-Γ-P-H|P-N

Body-centered cubic

H Corner point joining four edges
N Center of a face
P Corner point joining three edges

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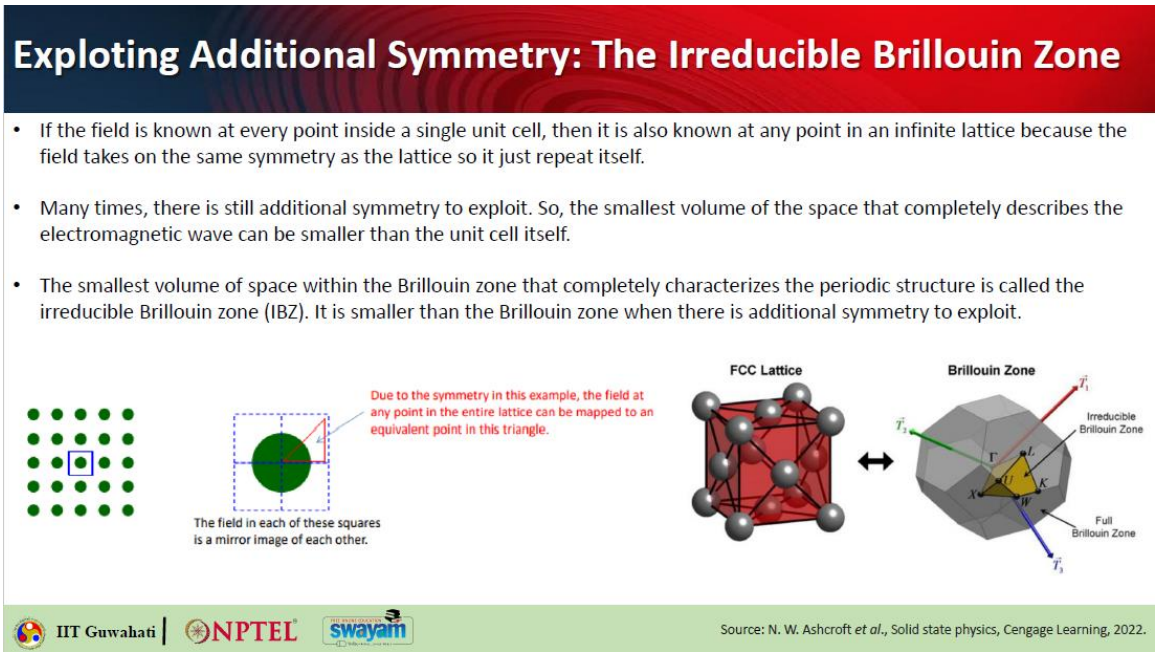
Source: N. W. Ashcroft *et al.*, Solid state physics, Cengage Learning, 2022.

So this particular volume will contain all the information of your Brillouin zone okay. You do not need to compute it for the entire region you can only compute it for this one. Similarly if you take hexagonal then these points gamma, K, M, L, H and A. So each of these points are defined here something I just read out 1 or 2 that M is basically the center of the rectangular phase. So, this is the rectangular phase, this is the center.

There is another phase here what is this phase? This is a hexagonal shape phase okay. So what is L? L is basically the middle of the edge that is joining the hexagonal shape phase and the rectangular shape phase. So, this point is L okay. What is H? H is basically the corner point. K is basically the midpoint of the edge that is joining two rectangular phases okay that is K as you can see here. So, these are the different irreducible Brillouin zones okay which are very very important for finding protonic band structure as well.



And if you take this simple shape cubic one and if you think only 2D. So you will only have gamma, M and X. So if you take a cross section like this that will make this structure a 2D. So you can only have gamma, M and X. Here also you can think of this is the hexagonal one, but if you take a 2D so you can get a 2D hexagonal lattice or this triangular lattice you can say.

So, there you have gamma, K, M and gamma. So, only this part will be in the 2D right. So that is the whole idea of having irreducible Brillouin zone as I mentioned that if this is your lattice and this is your unit cell okay. So, your objective would be to only find out the region that this region should replicate the entire one. So, if you take only this particular region as you have discussed before, if you take a flipped version of it here or rotate it here you can get this particular square and then you can use mirror on the other side to get this left one. So, once you have the upper half you can put a mirror here and you can get the entire structure.

So, it means if you only compute for this triangular region it will contain the same kind of information okay. Similarly in FCC lattice we have seen this is the Brillouin zone

which has got 14 it is a octahedral shape with 14 sides. In between if you actually identify this region which is the smallest volume of space within the Brillouin zone that completely characterizes the periodic structure is called the irreducible Brillouin zone. So, you cannot further reduce your Brillouin zone. So, this is the minimum portion of the Brillouin zone that is required to give you the overall property of the Brillouin zone okay and that is why it is called irreducible Brillouin zone and so two things here. So, this octahedral shape is the full Brillouin zone, this painted region here this volume is the irreducible Brillouin zone and this will help us in reducing the computational burden for finding out different modes and the photonic band structure for this particular crystal or crystals setup okay.

So, with that we will stop here today and in case you have any doubt you can write me to this email address mentioning MOOC on the subject line. Thank you.