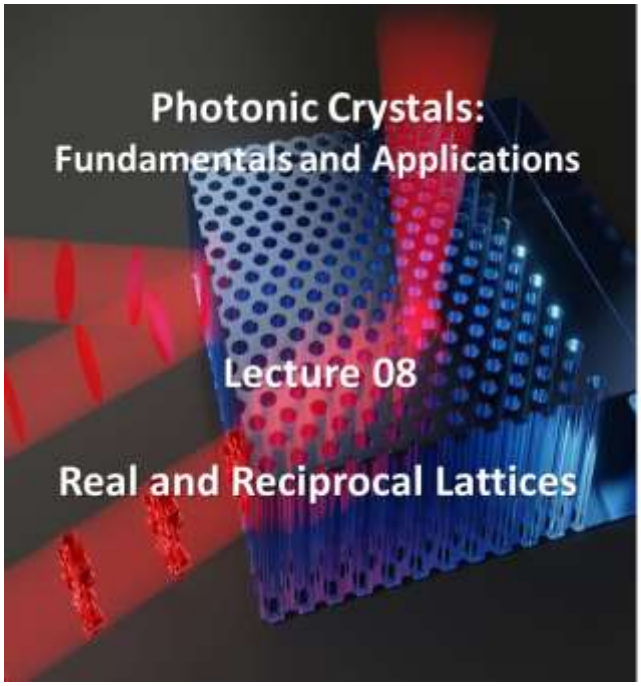


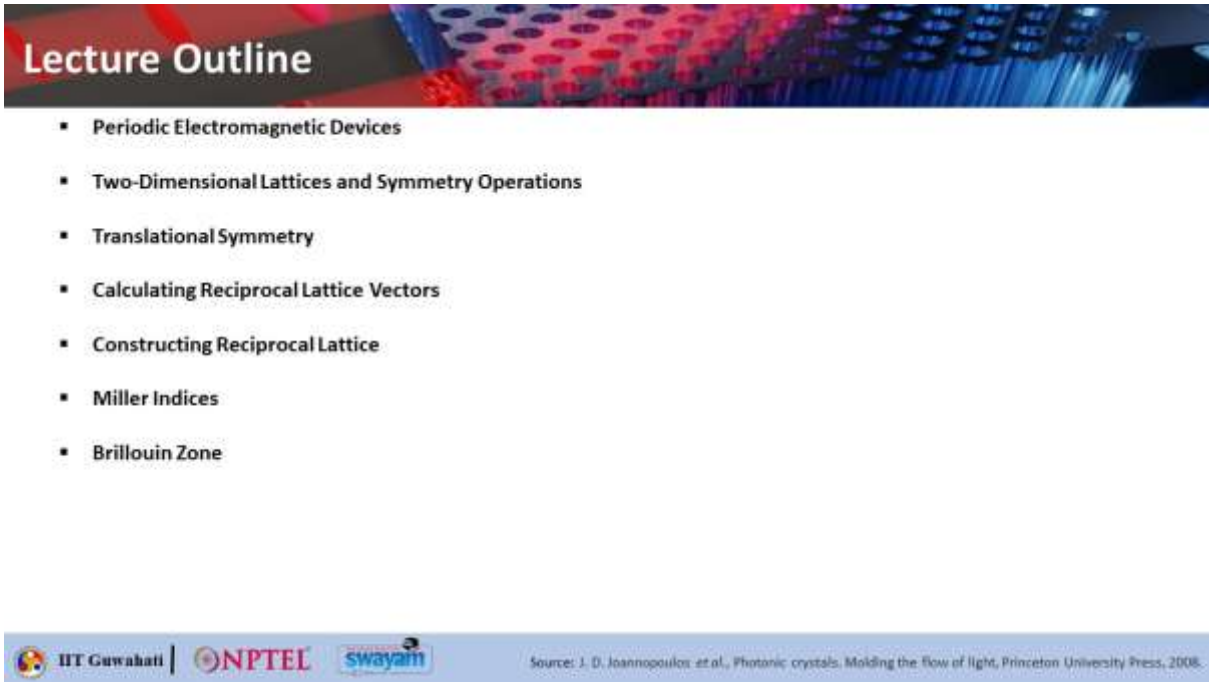
Dr. Debabrata Sikdar

Department of Electronics and Electrical Engineering
Indian Institute of Technology Guwahati

Web: https://www.iitg.ac.in/deb.sikdar
Email: deb.sikdar@iitg.ac.in

Lec 8: Real and Reciprocal lattices

Hello students, welcome to lecture 8 of the online courses on Photonic Crystals, Fundamentals and Applications. Today's topic will be on Real and Reciprocal Lattices



So, here is the lecture outline. We will discuss about Periodic Electromagnetic Devices into the details of two-dimensional lattices and the symmetry operations. Briefly touch upon translational symmetry or discrete translational symmetry which is relevant to the study of photonic crystals. We will look into the calculation of reciprocal lattice vectors, constructing reciprocal lattice, finding out the Miller indices obtaining brilliant zone and then irreducible brillouin zone ok.

Periodic Electromagnetic Devices

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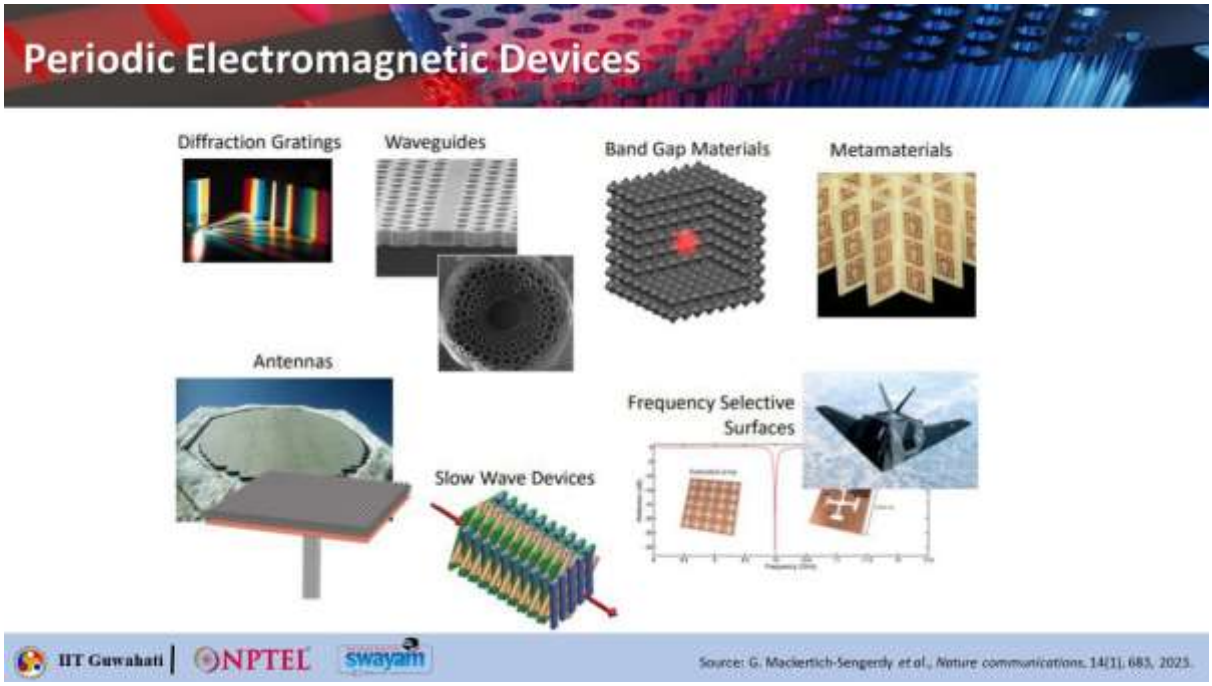
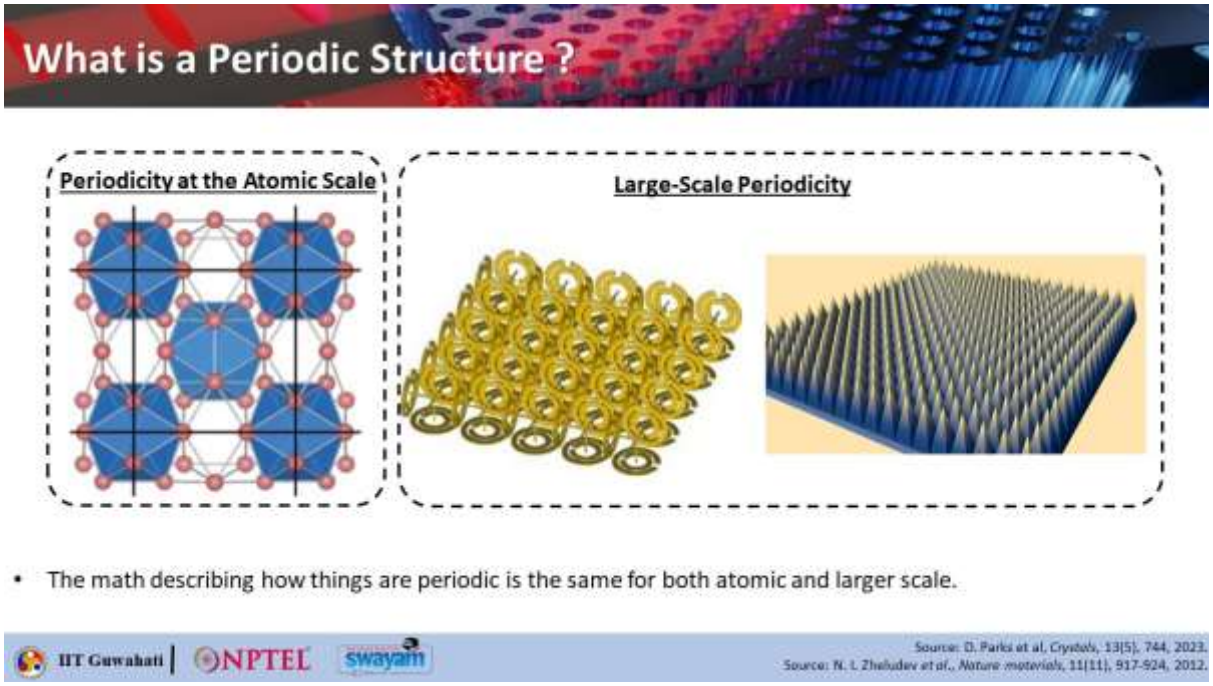
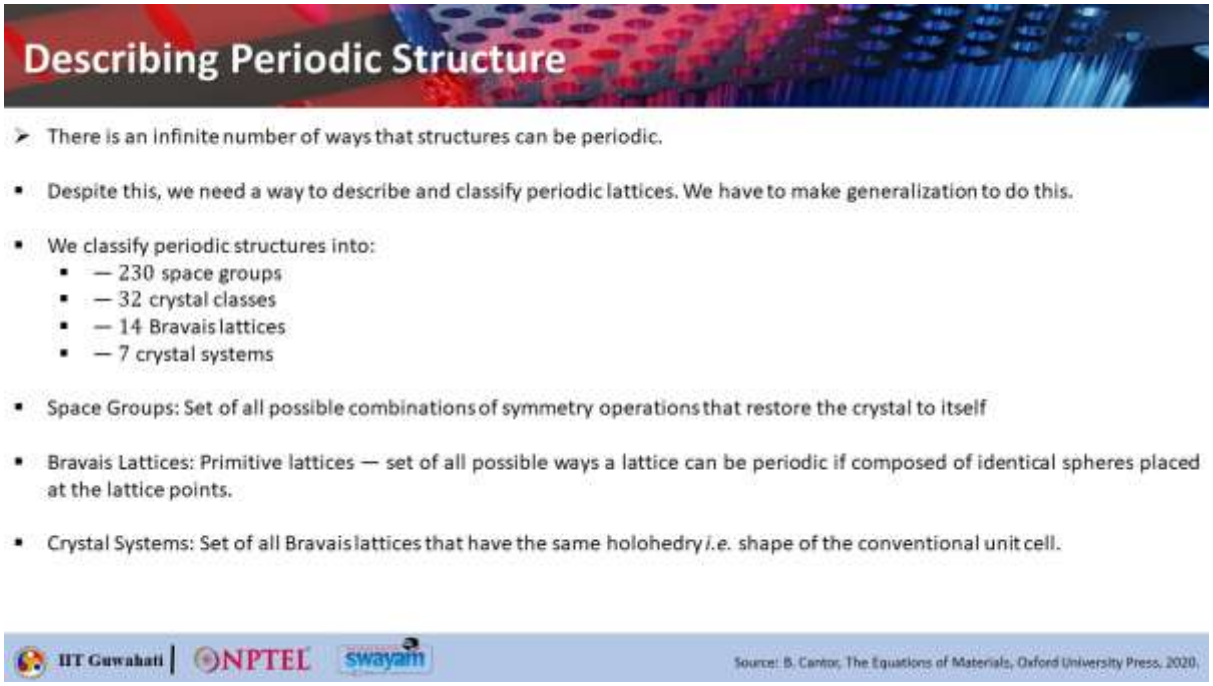


So, let us first discuss periodic electromagnetic devices. As you can see on this particular slide there are different types of you know periodic electromagnetic devices are shown here starting from diffraction grating to waveguides wholly photonic bandgap fiber, you have band gap materials, metamaterials, then periodic array antennas, slow wave devices and frequency selective surfaces. So, these are all periodic devices where the property is mainly defined by the unit cell and the periodicity



So, what is a periodic structure? So, here you can see periodicity at atomic scale.

So, these are different atoms, okay. And if you try to replicate this in your engineering design, where you make one-unit cell and then try to repeat it periodically, you can actually get large scale periodicity, something like this or this. So, what is fundamental here is that the math which describes the periodicity in atomic scale or large-scale periodicity both are similar. So, let us look into how we can describe periodic structures. So, there is an infinite number of ways a structure can be periodic.

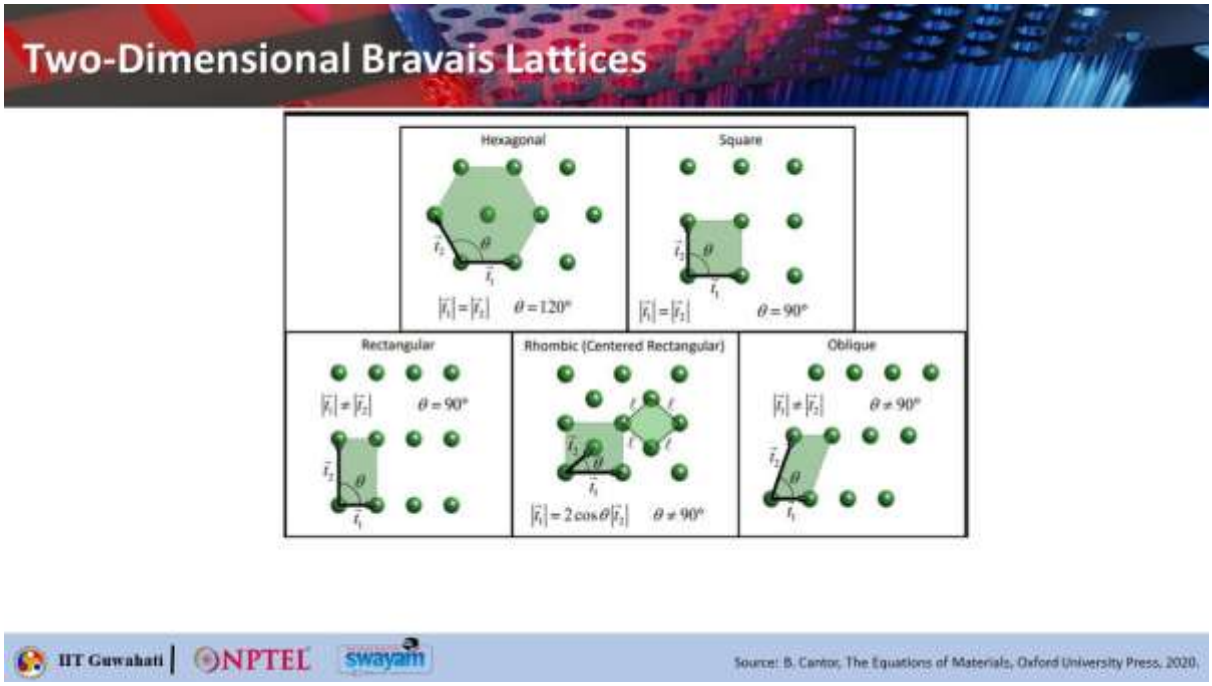


Despite this, we will need to find a way to describe and classify these periodic lattices. So, we have to make some generalization to achieve that. So, we can classify periodic structures into 230 lattice into 230 space groups, 32 crystal classes, 14 Bravais lattice and 7 crystal systems. Space group are basically the set of all possible combinations of symmetry operations that could restore the crystal to itself. So there are too many 230 space groups so we do not deal typically with space groups.

How about Bravais lattice? Yes. So, we mainly focus on Bravais lattice and the seven crystal systems. So, if you look into Bravais lattice, you can see that the primitive lattices are set of all possible ways a lattice can be periodic. If composed of identical spheres which are basically placed at the lattice points. You can also consider you know the set of all Bravais lattices okay which have the same hollowheadry or you can say the same shape of conventional unit cell you can group them into crystal systems.

That is why we have 14 Bravais lattices and we have 7 crystal systems. So, let us take some examples and find out you know how do you apply all this fundamental concepts on 2 dimensional lattices and also look into the symmetry operations which are possible

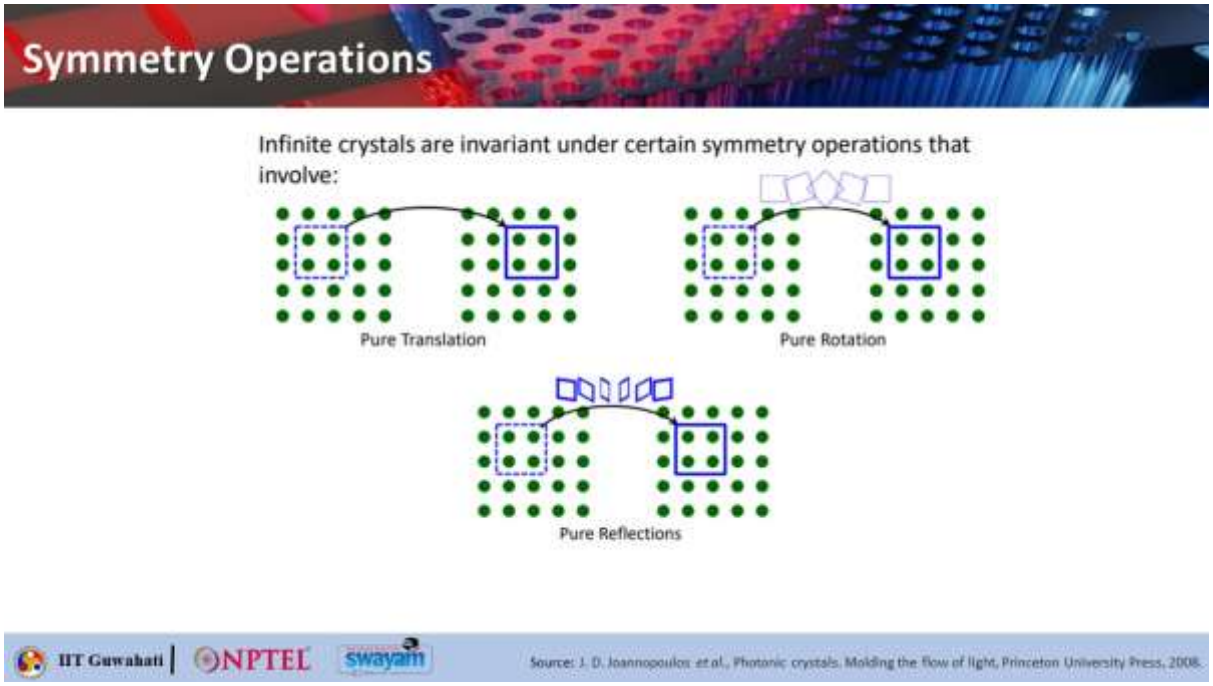
Two-Dimensional Lattices and Symmetry Operations



So, here are some examples of two dimensional Bravais lattice. You can see here this is a hexagonal lattice where the atoms or the unit cells you can say they are all arranged in a hexagonal array. They can also so when you say a hexagonal array these two vectors t1 and t2 are basically same but of equal length but the angle between them will be 120 degree okay.

So, in case of square you can understand that the lattice is basically square. So, the distance from here to here and here to here will be same again. So, you can say modulus of T1 vector and modulus of T2 vector will be equal and in this case the angle between them theta is equal to 90 degree. You can also think of rectangular lattice where T1 and T2 will not be equal, but they will maintain that 90-degree angle. you can think of rhombic lattice like this where you can have this kind of length L forming a diagonal pattern.

So, here basically T1 is considered to be twice cos theta times T2. okay and the angle is definitely not 90 degree. So, these are different lattice types you can also have oblique lattice where t1 and t2 are not equal and again you know angle theta between these two vectors is not 90 degree. So, you can understand the difference between this rhombic and oblique Bravais lattice.

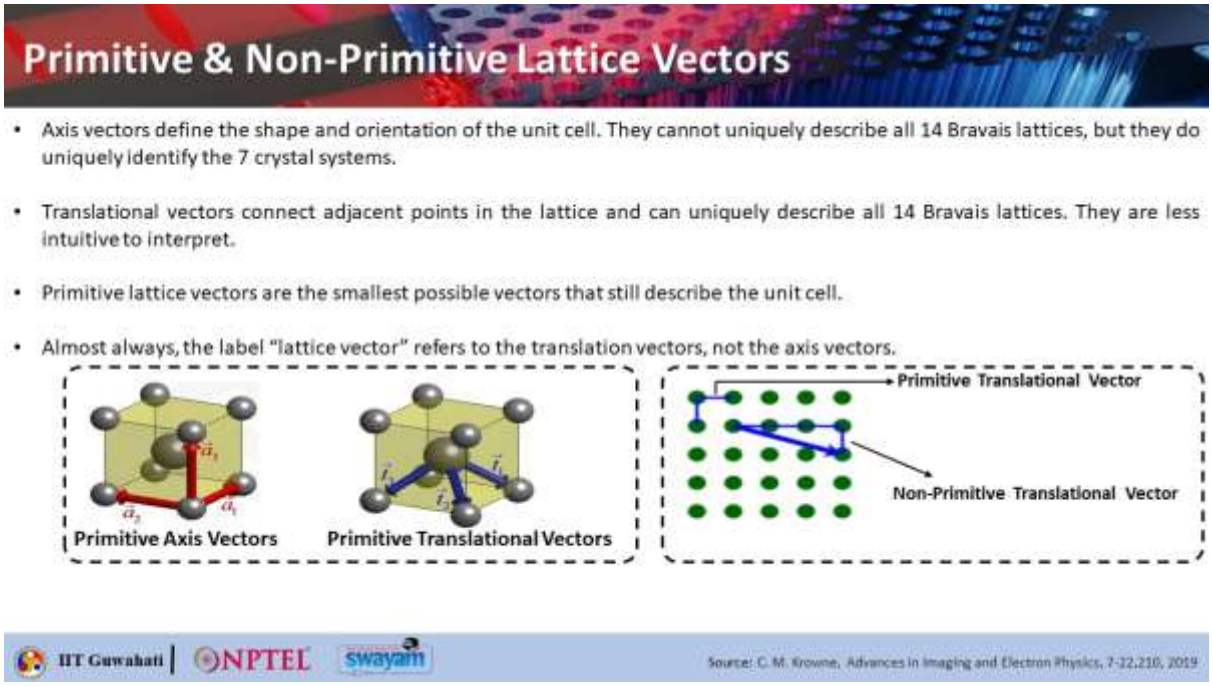


Now, we will look into the symmetry operations that can be performed on Bravais lattice.

So, the type of symmetry in which an object moves from one position to another position with the same orientation okay, So, in forward or backward motion that kind of symmetry is called translation. So, you can actually think of this moving forward or backward and that will actually replicate the same part of the crystal. So, you can think of this infinite crystal to be invariant under translation operation. Similarly, you can also think of rotational symmetry, which is the symmetry in which an object fits into itself while being rotated through 360 degrees. So, if you take this one and rotate these 360 degrees, you see it actually comes back to itself.

Okay. So, these are the kind of steps you can think of. Right. And another type of symmetry is reflection symmetry. Right. So, here you can see it is a type of symmetry in which a line could divide an object into two coincidental parts.

So, if you can think of a line here, this part, the left and the right part are basically mirror image of each other. So, it actually has got the mirror symmetry. right or the reflection symmetry. So, with that we will now describe the primitive and the non-primitive lattice vectors. So, the axis vectors okay will help us to define the shape and orientation of the unit cell and a unit cell is very important in case of any periodic structure because that unit cell contains all the properties okay and then it will be repeated periodically along you know 1 dimension, 2 dimension or 3 dimensions depending on whether you are talking about 1D, 2D or 3D periodic structure.

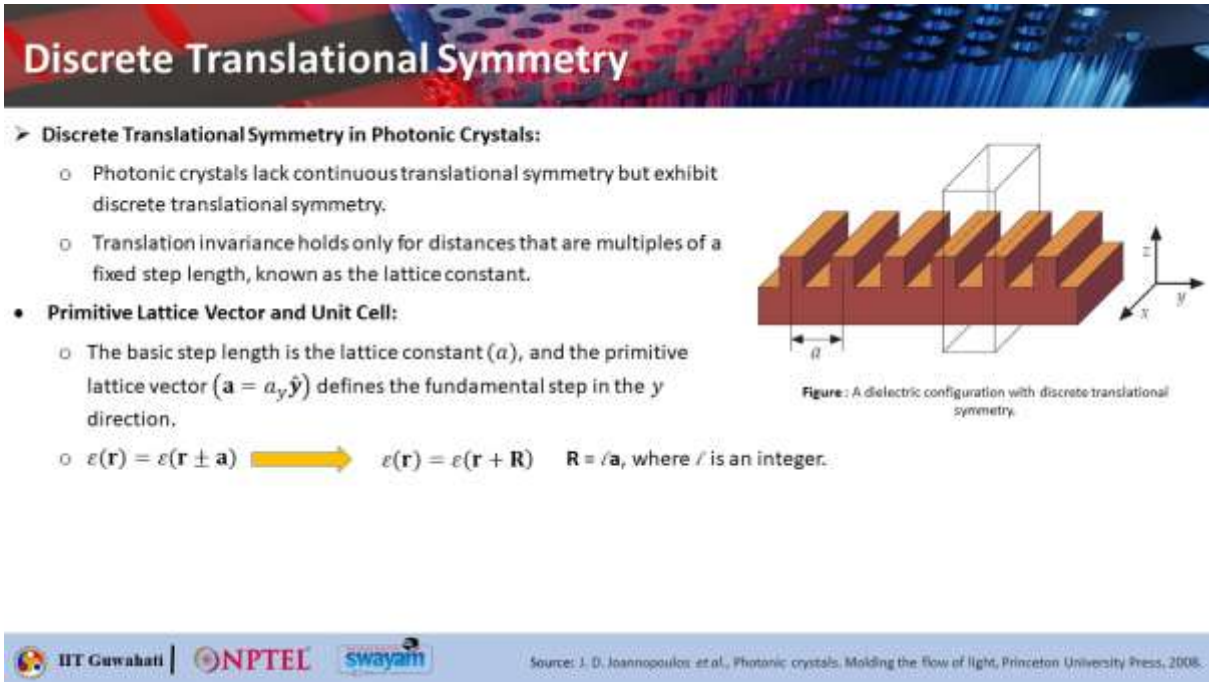


So here you can see that you know this axis vectors they cannot uniquely describe 14 Bravais lattice but what they can do they can uniquely describe the 7 crystal systems. So, you can also think of translational vectors like this T1, T2 and T3, okay, which connect the adjacent points in the lattice and this can be used for describing the 11 Bravais lattice systems, okay. So, this you can understand that this one is same for this BCC as well as simple cubic, right, and also for FCC. So, this kind of structure so that is why you know the primitive axis vectors cannot uniquely describe 14 Bravais lattice, but they can do the crystal systems ok

So, here you can see that when you talk about primitive lattice they are basically the smallest possible vectors that can describe the unit cell.

almost always when we use the level of lattice vector that refers to the translational vectors like this. We do not talk about the primitive axis vectors right and this is not the smallest one. So, this will not be considered as a primitive translational vector. So, the primitive translational vector is basically the smallest possible vector ok.

Translational Symmetry



So, here we bring back again the description or discussion about discrete translational symmetry, okay, which you can see in case of this 1D photonic crystal that is shown here and this particular black box, this thin box marks the unit cell, right.

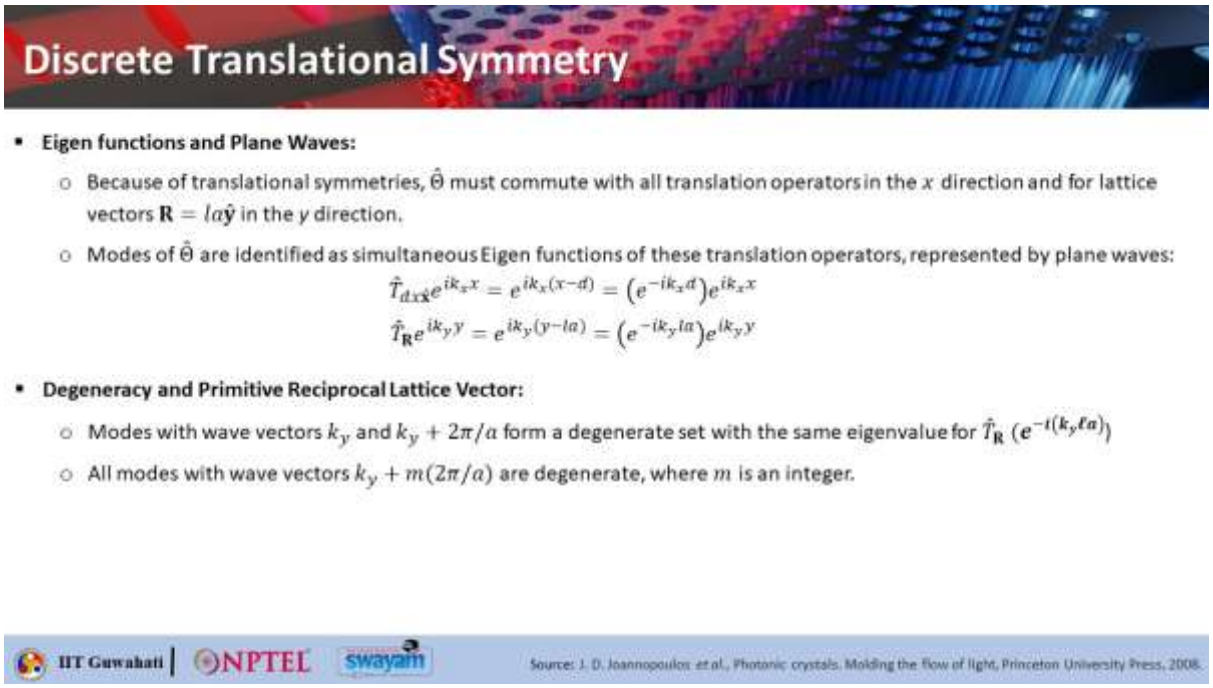
So, why is this important? It is important because photonic crystals lack continuous translational symmetry, but they exhibit discrete translational symmetry. And it means that the translation invariance holds only for distances which are basically multiple of a fixed step length or that is also known as the lattice constant. So, if you take you know the if this is the lattice constant and you know in integral multiple of this lattice constant you will see that the feature is basically repeating. So, it has got this discrete translational symmetry. Now because of this discrete translational symmetry okay you can also write that you know the lattice vector A is basically A y by cap because here you can see that the periodicity is extended along the y direction okay and you can also write that epsilon r as epsilon r plus minus a.

So, this is true but then it also repeats for all the integral multiple of a. So, it is better to be written as epsilon r equals epsilon r plus capital R where capital R is basically L a where L is an integer. right. So, that way you can understand that discrete translational symmetry exists in the photonic crystal. Now, because of the translational symmetry we have seen in the previous lecture also that the Maxwell's operator theta cap okay must commute with all translational operators in the x direction and for lattice vectors capital R which lie in the y direction and R as you have seen it is basically represented as L A y cap what is L it is an integer A is the lattice constant.

So, the modes of theta cap are identified as the simultaneous eigen functions of this translational operator represented by the plane waves which can be expressed like this okay. So, the first equation here shows the continuous translational operator where you are moving the system by a displacement of d. But, in this case for the periodic crystal or for the periodic system, so dx is now

replaced by capital R where capital R is basically integral multiple of the lattice constant A. So, you can also see d is replaced by this okay. So, this way you can actually see the eigen function okay which is represented by the plane waves.

So, what we understand here that the modes with wave vector k y and k y plus 2 pi by a they will form a degenerate set with the same eigenvalue of T r e to



Calculating Reciprocal Lattice Vectors

Calculating Reciprocal Lattice Vectors

- The impermeability $\eta(x, y) = \epsilon_a/\epsilon(x, y)$ is periodic in the transverse directions, x and y, and uniform in the axial direction z.

$$\eta(x + m_1 a_1, y + m_2 a_2) = \eta(x, y) \qquad \text{(L8.1)}$$

for all integers m_1 and m_2.

$$\eta(x, y) = \sum_{\ell_1=-\infty}^{\infty} \sum_{\ell_2=-\infty}^{\infty} \eta_{\ell_1,\ell_2} \exp(-j\ell_1 g_1 x) \exp(-j\ell_2 g_2 x) \qquad \text{(L8.2)}$$

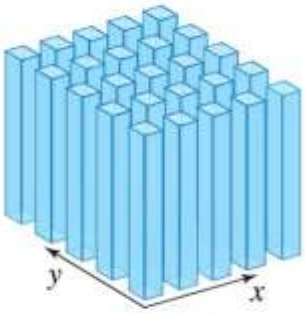


Figure: Rectangular Lattice.

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

So, in this kind of a system we can think of the impermeability parameter which is $\eta(x, y)$ that is basically $\epsilon \quad \epsilon$. So, this impermeability is periodic in the transverse direction x and y and it is basically uniform along the axial direction that is z. So, you can also write if you consider a1 and a2 as the periods in x and y direction okay. So, this is a rectangular lattice. So, the period here is a1 and a2 okay.

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.

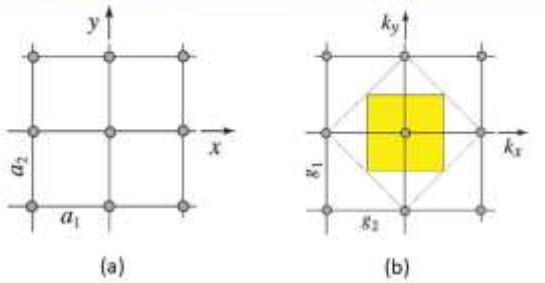


Figure: (a) The rectangular lattice at which the rods are placed. (*b*) The two-dimensional Fourier transform of the lattice points is another set of points forming a reciprocal lattice with periods $g_1 = 2\pi/a_1$ and $g_2 = 2\pi/a_2$.

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

Then $\eta(x, y)$ will also satisfy the translational symmetry like this okay. anything in place of x you can write $x + m_1 a_1$ for y you can write $y + m_2 a_2$ and that the property should repeat itself. The impermeability should repeat itself and that is how this is a periodic rectangular lattice. Now this periodic function $\eta(x, y)$ can be represented as a two-dimensional Fourier series in this particular form where you can say you know l1 ranges from minus infinity to infinity then you have summation over l2 ranging from minus infinity to infinity eta l1 l2 exponential minus j l1 g1 x times exponential minus j l2 g2 x. So, what are this g1 and g2? So, $g_1 = 2\pi / a_1$ and $g_2 = 2\pi / a_2$

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.

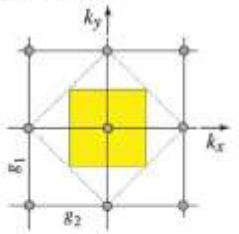


Figure: Reciprocal Lattice (The shaded (yellow) area is the Brillouin zone).

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

These are the fundamental spatial frequencies. The units are radian per millimeter, okay. So, these are the spatial frequencies in the x and y direction and l1 g1 and l2 g2 are basically their harmonics. So you can think of this one here. So this is the rectangular lattice in which the rods are placed.

Here we have shown them with circles. You can also imagine squares because if you consider the previous figure, they are having square cross-section. So the period along x is a_1, the period along y is a_2. okay. And this is the two-dimensional Fourier transform of this lattice points okay.

So, you are changing from the x space to k space. So, here you can see the coordinates have changed to k x and k y and this is basically the reciprocal lattice of this one which has got periods of g 1 ok, which is $2\pi / a_1$ and g 2 equal to $2\pi / a_2$. So, this is the real lattice and this is the reciprocal lattice. So, we understood that this is the Fourier domain load lattice which is known as reciprocal lattice as the convention of solid state physics right. Now, in this kind of case what are the optical modes of a medium with this kind of with such symmetry.

So, we can consider for waves travelling in the direction parallel to xy plane. The modes are basically two dimensional block waves. So, you can write you know $U(x,y) = p_{K_x,K_y}(x,y)\exp\left(-jK_x x\right)\exp\left(-jK_y y\right)$. So, what are this $p_{K_{x'}}$ and p_{K_y} they are basically you know the periodic function with the same period as the medium. So this is how the you know this is the two dimensional block wave it means you know the wave will also pick up the periodicity of the crystal.

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**.

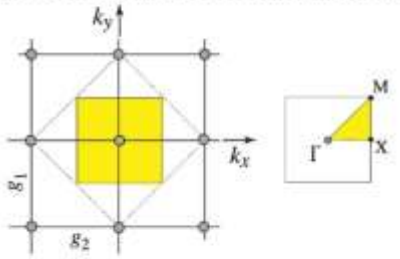


Figure: Reciprocal Lattice. For a square lattice ($a_1 = a_2 = a_3$), the irreducible Brillouin zone is the triangle ΓMX.

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

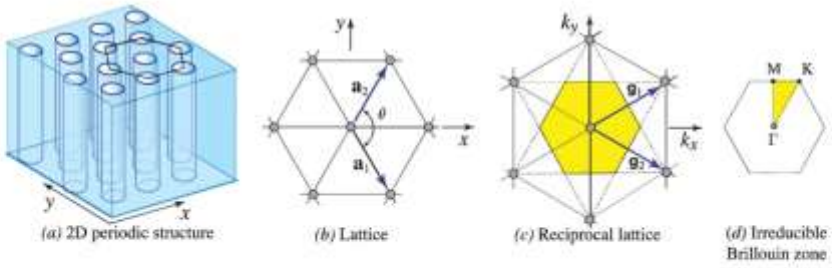
And as you can see this wave is basically specified by a pair of block wave numbers kx and ky okay. So, another wave with block wave number $K_x + g_1$ comma okay this will be k2, $K_x + g_2$ will not be a new mode okay it will be rather the same mode right. So, here you can see that a complete set of modes in the Fourier plane has block wave numbers located at points in the rectangle shown in yellow which is basically defined between now kx within minus g1 by 2 to g1 by 2 and ky between plus gy plus g2 by 2 and So, k y will be from minus g 2 by 2 to g 2 by 2 right. So, as shown in the figure a complete set of modes in the Fourier plane has block wave numbers located at the points in the rectangle which is shown in yellow and this rectangle is defined by the boundaries of k x So, kx will be from minus g1 by 2 to g1 by 2 and k2 will be from minus g2 by 2 to g2 by 2 okay and that dictates the first Brillouin zone. So, when you think of this yellow square or a rectangular area as the first Brillouin zone ok.

So, you may think of all the independent block wave vectors are basically captured here, but there may be a lot of you know redundant ones. So, if you try to use the symmetry to further reduce the set of independent block vectors within this Brillouin zone what you will get you will basically come up with an area like this a triangle which is called the irreducible Brillouin zone. So, here you will find all the independent block wave vectors which can be used to recreate this Brillouin zone. For example, if you use rotational symmetry which is inherent to this square lattice okay you can see that the irreducible Brillouin zone can be rotated and folded here. So, you get this particular quarter then again you can do the mirror of it you will get this first half and then you take a mirror operation like this you can complete this entire square.

Calculating Reciprocal Lattice Vectors

- A two-dimensional periodic structure comprising parallel cylindrical holes. The triangular lattice at which the holes are placed. In this diagram the magnitudes $a_1 = a_1 = a$ and $\theta = 120°$.

- Reciprocal lattice — the shaded (yellow) area is the Brillouin zone, a hexagon. The irreducible Brillouin zone is the triangle ΓMK.



(a) 2D periodic structure (b) Lattice (c) Reciprocal lattice (d) Irreducible Brillouin zone

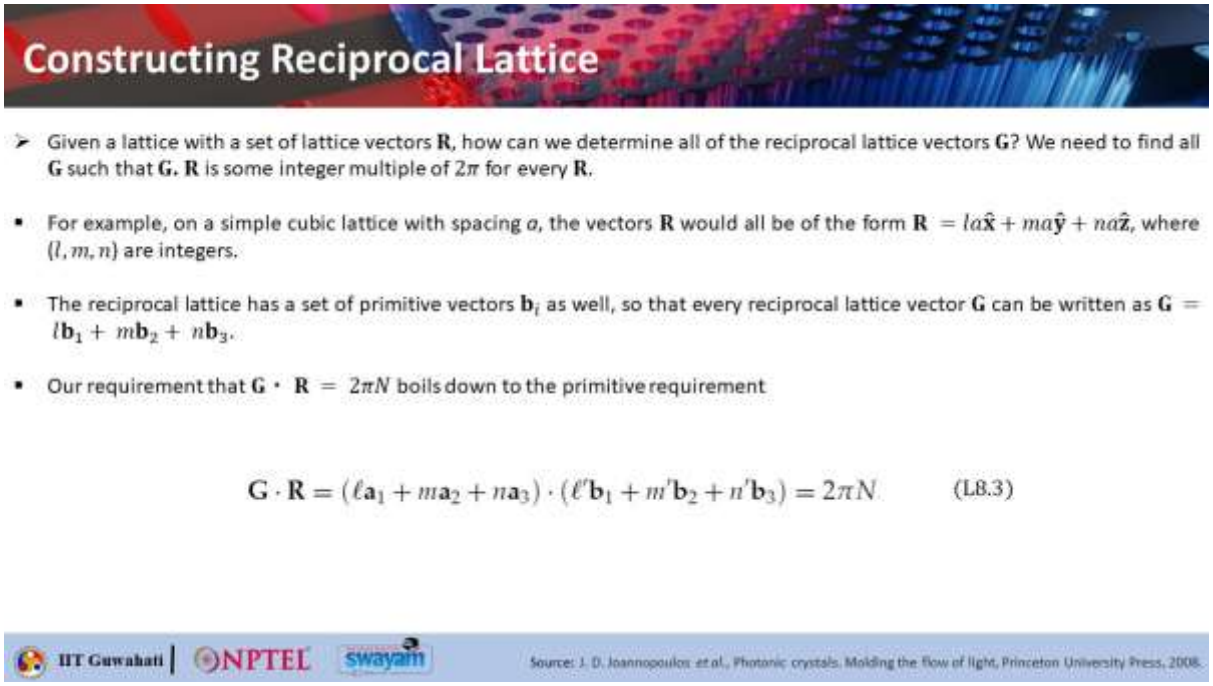
IIT Guwahati | NPTEL swayam Source: B. E. Saleh and M. C. Teich, Fundamentals of photonics, John Wiley & Sons, 2019.

So, that way you can form the entire Brillouin zone from the irreducible Brillouin zone right. So in this irreducible Brillouin zone the triangle is marked as gamma mx as I mentioned for the square lattice these are the three important points. Now for calculating the lattice vectors okay What you can see here, so this is basically a two-dimensional periodic structure which is comprising of parallel cylindrical holes. And what is the lattice pattern here? The lattice pattern is triangular or hexagonal, okay. So, at those lattice points the holes are placed.

So, here from the figure you can say that A1 and A2 the two basic lattice vectors are basically equal okay and the angle between them is 120 degrees. Right. So when you try to take this into Fourier space, you convert x and y into kx and ky. And you can see that this yellow marked region is basically the Brillouin zone which is basically a hexagon. So, here again when you try to find out the irreducible Brillouin zone you can see that the you can find a triangle marked by gamma mk ok.

These are the three points which can mark the irreducible Brillouin zone. So, we will come into this that how do you obtain this reciprocal lattice by calculation. So, here is that topic of calculating or constructing irreducible sorry

Constructing Reciprocal Lattice

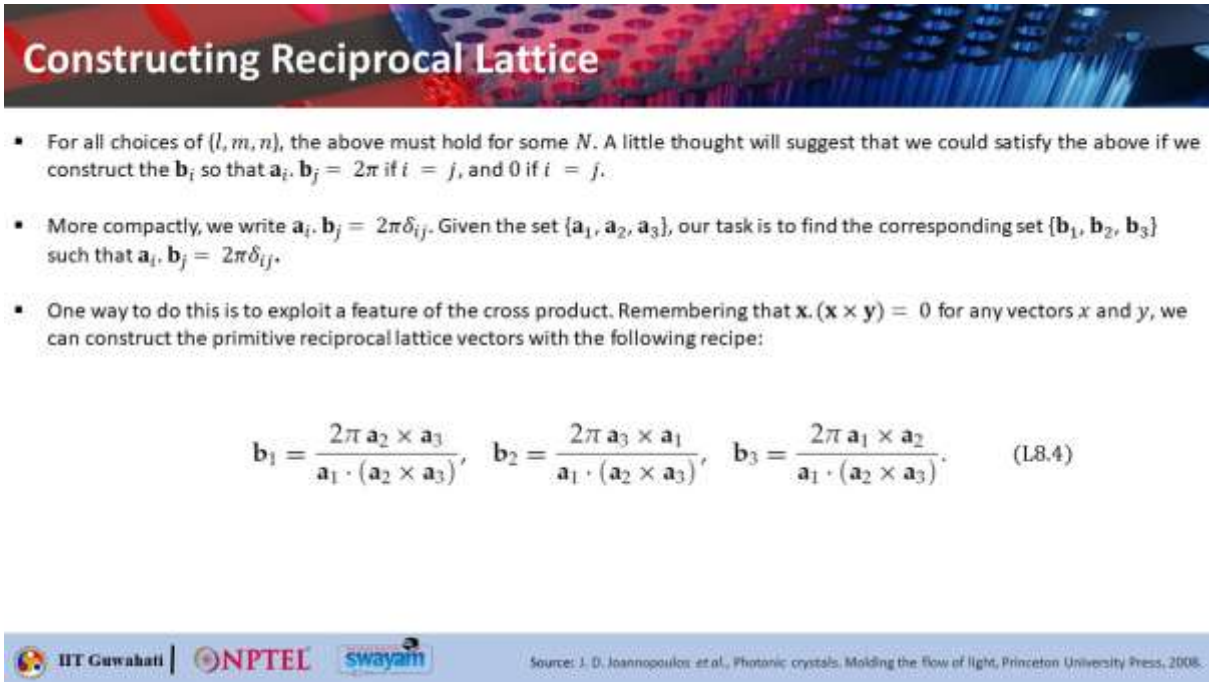


Now, let us see how do we construct the reciprocal lattice. So, given a lattice with the set of vectors lattice vectors capital R, our job is to now find out all the reciprocal lattice vectors which can be denoted as capital G.

So, we need to find all g such that g dot r is some kind of integer multiple of 2 pi for every r, right. Then only they will like satisfy the condition that they are reciprocal lattice factors. Now, for example on a simple cubic lattice with spacing of small a. okay the vectors r would all be of the form $\mathbf{R} = la\hat{\mathbf{x}} + ma\hat{\mathbf{y}} + na\hat{\mathbf{z}}$.

So, where l m n are basically integers right. So, we know that every lattice vector capital R can be written in terms of the primitive lattice vectors which are basically the smallest vectors pointing from one lattice point to another right. So, these are the lattice vectors right primitive lattice vectors. So, in the reciprocal lattice also they have the same set of you know similar set of primitive vectors you can name them as small bi okay. So, that every you know reciprocal lattice vector g can also be expressed as $G = l\mathbf{b}_1 + m\mathbf{b}_2 + n\mathbf{b}_3$ again L m n are integers right. So, what is the requirement? The requirement is that you know $\mathbf{G} \cdot \mathbf{R} = 2\pi N$ ok.

So, n is an integer again ok. So, this is the requirement that we discussed here. So, this boils down to the primitive requirement.



So, if you take the form that you have thought of ok. So, you can write g dot r. So, this is basically your r okay r vector l m n you can use different integers to represent that they are not necessarily the same one.

So, it can be $\left(\ell \qquad _2 + n'\mathbf{b}_3\right)$ and that should be equal to 2 pi n. For all choices of l m n as you have seen okay there this particular value should be true. Then only g is considered to be the reciprocal lattice vector of capital R. Now a little thought will suggest us that we could satisfy the above if we construct b i so that $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi$ if i and j are equal and there is it is 0 this product is 0 if they are not equal ok.

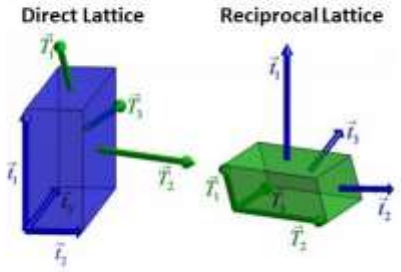
So, this one is not equal yeah. So, more completely you can basically write that $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi$ and then you have δ_{ij} right. So, this when i and j are equal δ_{ij} will be 1 when i and j are not equal it will be 0. So given the set, you have three vectors, A1, A2, A3. Our task is to find the corresponding set, B1, B2, B3, such that this particular condition is satisfied, that $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$. So, one way to do this is to exploit the feature of the cross product.

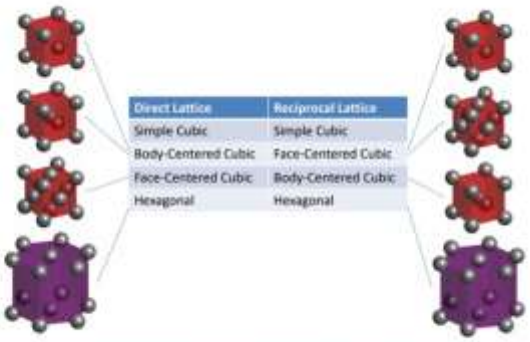
So if you remember that $\mathbf{x}.(\mathbf{x}\times\mathbf{y}) = 0$ for any vector x and y. So, you can construct the primitive lattice vectors using the following recipe. So, you can

$\mathbf{b}_1 = \frac{2\pi\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad \mathbf{b}_2 = \frac{2\pi\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \quad \mathbf{b}_3 = \frac{2\pi\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$. using this formula. So, that is how you can obtain b1 a1 from a1, a2, a3 you can find out what is b1, b2 and b3. So, to construct the reciprocal lattice what we do you first take the primitive lattice vectors a1, a2, a3 and then perform the operations using this formula and obtain b1, b2 and b3.

Constructing Reciprocal Lattice

- To construct the reciprocal lattice vectors, we take the primitive lattice vectors and perform the operations of equation (I.8.4).
- 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. Kroome, Advances in Imaging and Electron Physics, 7-22,210, 2019.

Direct to the Reciprocal

- The reciprocal lattice vectors can be calculated from the direct lattice vectors (2D and 3D).

2D

$$\vec{T}_1 = \frac{2\pi}{\left|\vec{t}_1 \times \vec{t}_2\right|}\begin{bmatrix} t_{2,y} \\ -t_{2,x} \end{bmatrix} \qquad \vec{T}_2 = \frac{2\pi}{\left|\vec{t}_1 \times \vec{t}_2\right|}\begin{bmatrix} -t_{1,y} \\ t_{1,x} \end{bmatrix}$$

$$\vec{t}_1 = \frac{2\pi}{\left|\vec{T}_1 \times \vec{T}_2\right|}\begin{bmatrix} T_{2,y} \\ -T_{2,x} \end{bmatrix} \qquad \vec{t}_2 = \frac{2\pi}{\left|\vec{T}_1 \times \vec{T}_2\right|}\begin{bmatrix} -T_{1,y} \\ T_{1,x} \end{bmatrix}$$

3D

$$\vec{T}_1 = 2\pi\frac{\vec{t}_2 \times \vec{t}_3}{\vec{t}_1 \bullet \left(\vec{t}_2 \times \vec{t}_3\right)} \qquad \vec{T}_2 = 2\pi\frac{\vec{t}_3 \times \vec{t}_1}{\vec{t}_1 \bullet \left(\vec{t}_2 \times \vec{t}_3\right)} \qquad \vec{T}_3 = 2\pi\frac{\vec{t}_1 \times \vec{t}_2}{\vec{t}_1 \bullet \left(\vec{t}_2 \times \vec{t}_3\right)}$$

$$\vec{t}_1 = 2\pi\frac{\vec{T}_2 \times \vec{T}_3}{\vec{T}_1 \bullet \left(\vec{T}_2 \times \vec{T}_3\right)} \qquad \vec{t}_2 = 2\pi\frac{\vec{T}_3 \times \vec{T}_1}{\vec{T}_1 \bullet \left(\vec{T}_2 \times \vec{T}_3\right)} \qquad \vec{t}_3 = 2\pi\frac{\vec{T}_1 \times \vec{T}_2}{\vec{T}_1 \bullet \left(\vec{T}_2 \times \vec{T}_3\right)}$$

- All reciprocal lattice vectors must be an integer combination of the primitive reciprocal lattice vectors.

$$\vec{T}_{hkl} = P\vec{T}_1 + Q\vec{T}_2 + R\vec{T}_3 \qquad \begin{aligned} P &= \cdots, -2, -1, 0, 1, 2, \cdots \\ Q &= \cdots, -2, -1, 0, 1, 2, \cdots \\ R &= \cdots, -2, -1, 0, 1, 2, \cdots \end{aligned}$$

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

So, with that you can actually understand that each direct lattice has a unique reciprocal lattice. So, the knowledge of one lattice will definitely tell you about the other lattice. So here you can see that the direct lattice vectors they are using a different notation. They are using small t okay as the notation for the direct lattice vectors, small t1, small t2 and small t3 okay. and they actually look like this when you see this in the reciprocal lattice.

But capital T1, T2 and T3 are the primitive vectors in the reciprocal lattice. So, there has to be some relationship between this small t1 and capital T2 and T3 with capital T1 and so on. So if you try to understand some of the commonly known lattice, so if you take simple cubic as a direct lattice, its reciprocal lattice is also a simple cubic. For BCC, or body centered cubic kind of lattice. The reciprocal lattice is a FCC face centered cubic and for FCC if you look into the reciprocal lattice it is a BCC, for hexagonal it is again hexagonal.

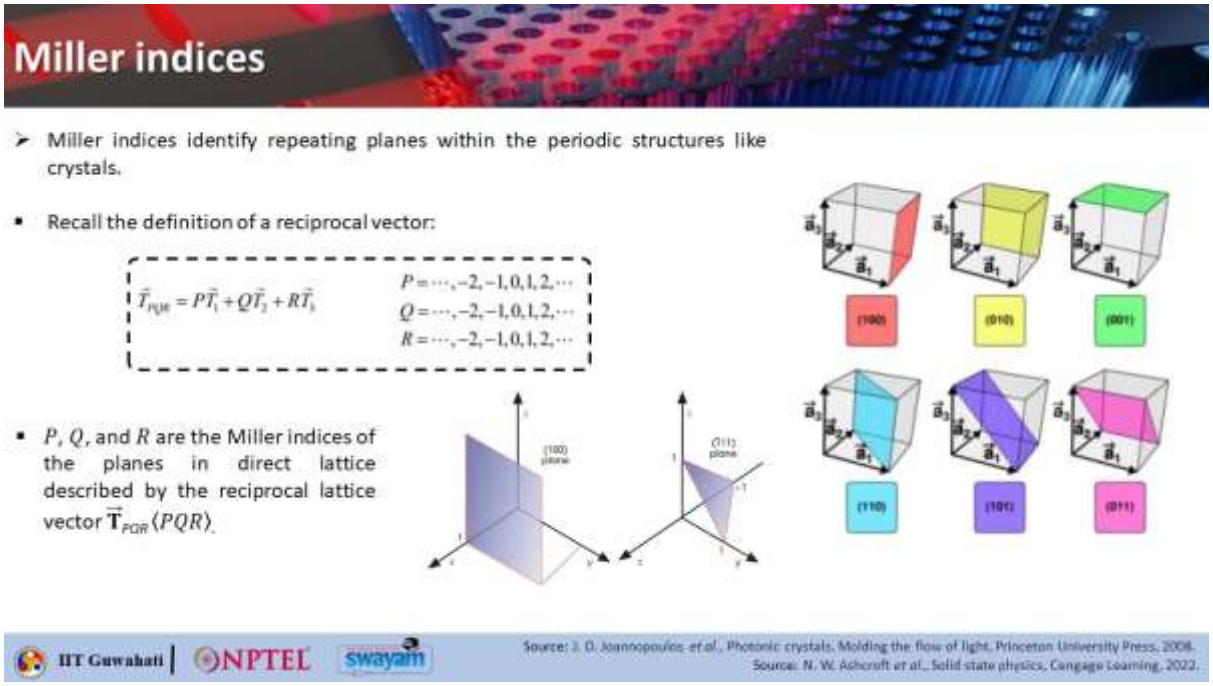
So, this is how a hexagonal lattice looks like, this is how a FCC looks like and this is how a BCC crystal looks like ok. So, the blue color ones tell you about the direct lattice vectors. So, this is in 2D it means you just have only 2 vectors t1 and t2. So, if you have small t1 and t2 known you can find out what is capital T1 and capital T2 ok. And also other way if you know the capital T1 and capital T2 you can find out what is small t1 and small t2 ok.

These are just different notations other than using A, B and C you can also use capital T1, T2, right. For 3D, it is like this. So, this is the formula that we have seen there, you remember.

So, B1, so this you if you take this formula. ok. This is exactly same as this one ok. These are like just different notations. So, different books follow different conventions. So, I am just showing you the different two most common notations used in this kind of calculations ok. So, you can find out what is capital T1, capital T2 and capital T3 right.

So, all reciprocal lattice vectors must be an integer combination of the primitive reciprocal lattice vectors that makes sense because the final vector capital G is basically integral times of the ah reciprocal primitive reciprocal lattice vectors. So, instead of G you can write capital T and you can say that the integer con ah capital P Q and R are basically the integers. So, you can write like this okay and capital T 1 bar T 2 bar and T 3 bar these are the primitive reciprocal lattice factors.

Miller Indices



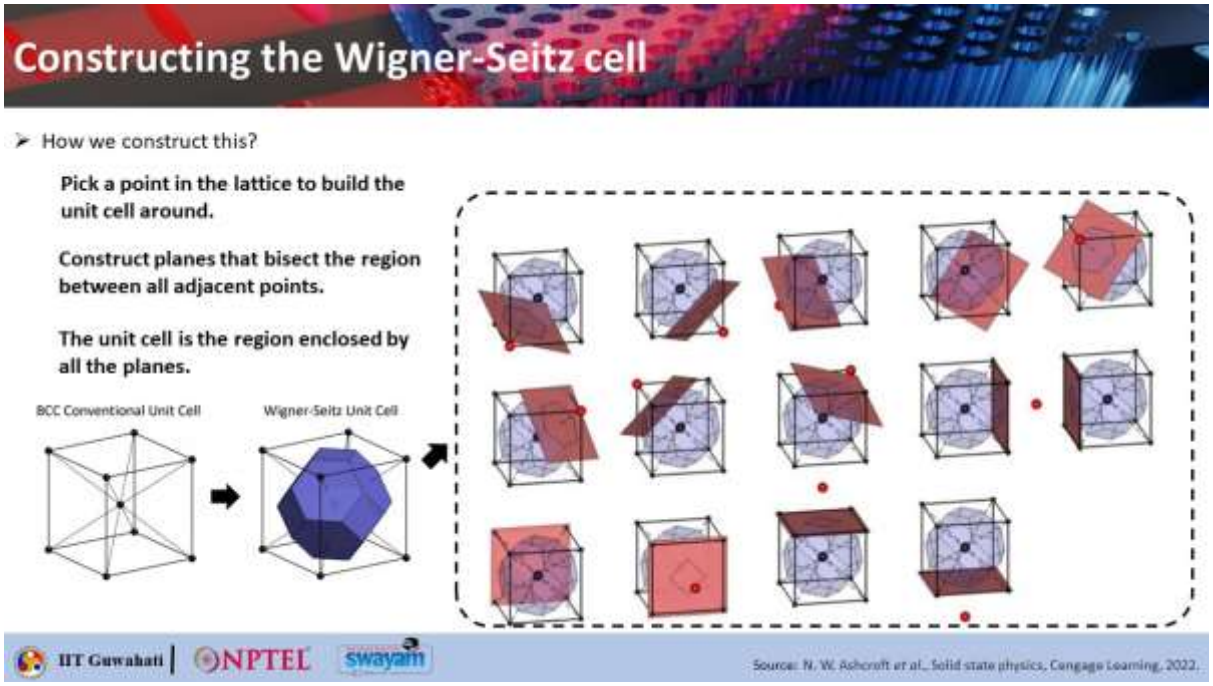
Now let us look into Miller indices that is another interesting way of representing planes within periodic structures like crystals. So, if you recall the definition of the reciprocal lattice vectors you have these three integers p, q and r ok.

So, this p, q and r are basically called the Miller indices of the planes in direct lattice which is represented by the reciprocal lattice factor t p q r and you can also represent it like this. So, if you say 1 0 0 plane it means it is 1 here it is a the plane is basically having an intersection or it is crossing the x axis at 1. and it is 0 0 means it does not intersect y and z axis.

So, it is parallel ok. So, 1 0 0 plane is typically like this. If you have 1 1 1 plane ok. So, it is basically intersecting x y and z at 1 1 1 ok. So, this one is basically x bar ok.

So, I think it is not clearly written. So, it is basically x bar ok. So, x bar means x bar means minus 1. So, this plane has got a cross section with the x axis at minus 1 and then it is crossing this y axis at 1 z axis at 1. So, it is 1 bar 1 1 plane ok. So, in such method you can think of 1 0 0 at this plane again this is another notation a 1 instead of using x y z you can also put a 1 bar a 2 bar and a 3 bar ok.

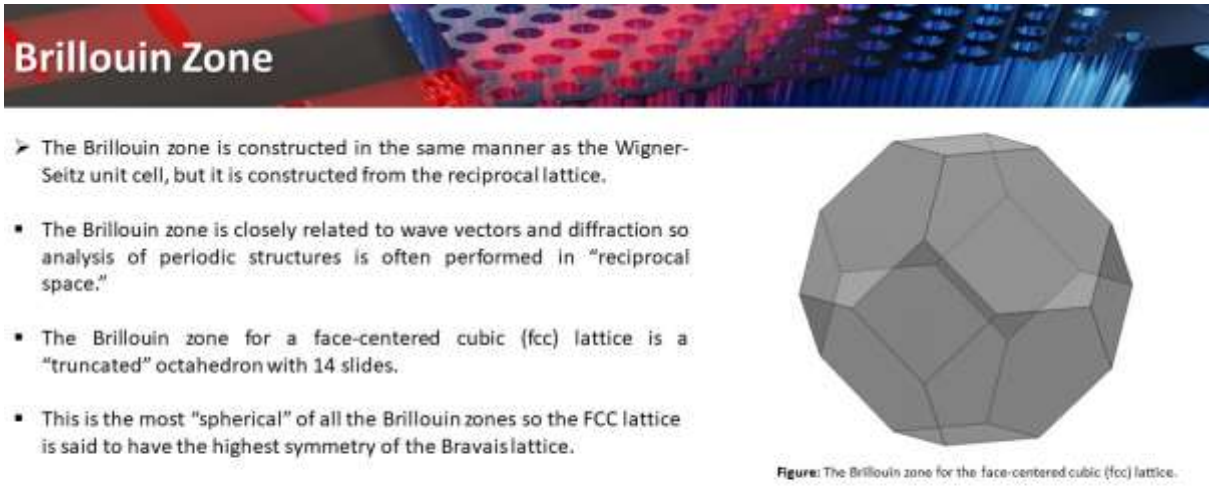
These are basically the direct lattice ok planes ok. So, 1 0 0 0 1 0 0 0 1 ok 1 1 0 will look like this 1 0 1 will look like this and 0 1 1 will look like this. And you can also think of how 1 1 1 will look like. So, it will have a you know cross section with A like this. So, the plane will typically look like this fine ok.



So, now let us first see how do you construct the Wigner shade cell. So, how do you construct this ok and why it is required. So, first you have to pick a point in the lattice to build a unit cell around it ok. So, this is the BCC conventional unit cell ok. Now, you construct planes that bisect the region between all adjacent point. So, if you take this and these two points, this point and this point, so there will be a plane.

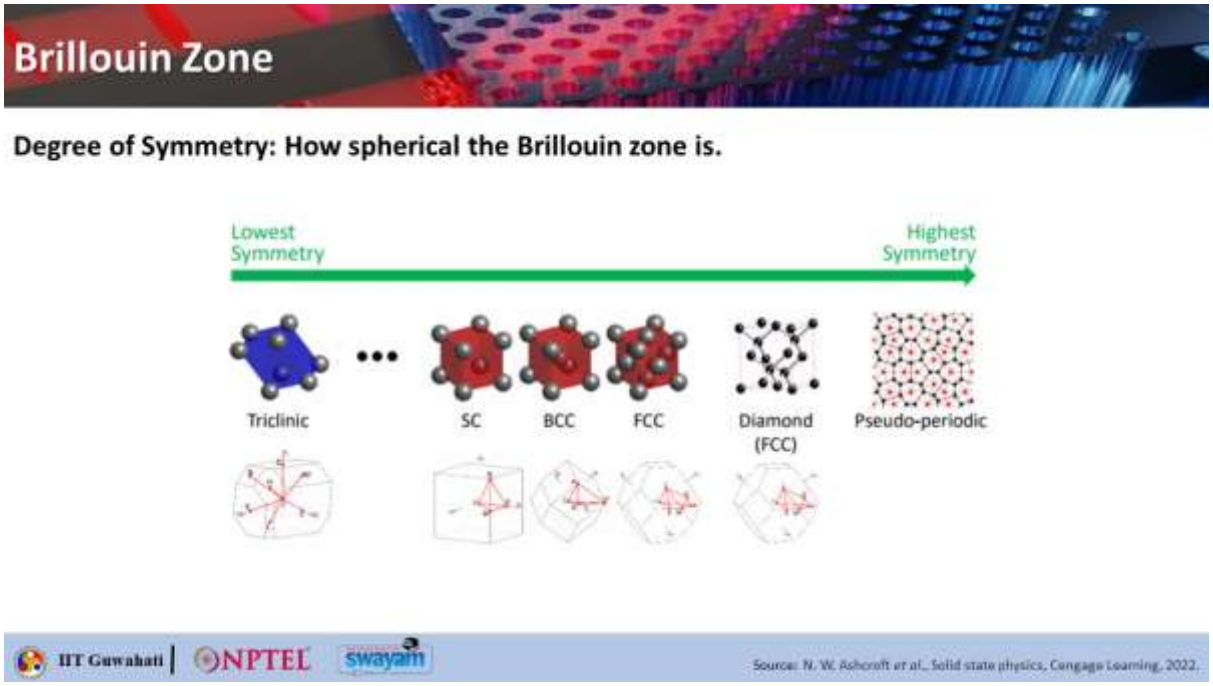
I am just drawing a line, but you think of a plane, it is basically this plane, ok. This plane which bisect that particular region and similarly you do it for all these connecting lines okay so wherever you have two adjacent points you are basically drawing a plane that bisect the region between the two adjacent points and when you add up all those points you basically get this wigner shades unit cell So, this is how you got to draw it. So, you take this and this one as I mentioned you take the you draw the connecting line and then you draw a plane that perfectly bisects that line or you can say it bisects that region between this point and this point. And then you repeat for all those possibilities.

Brillouin Zone

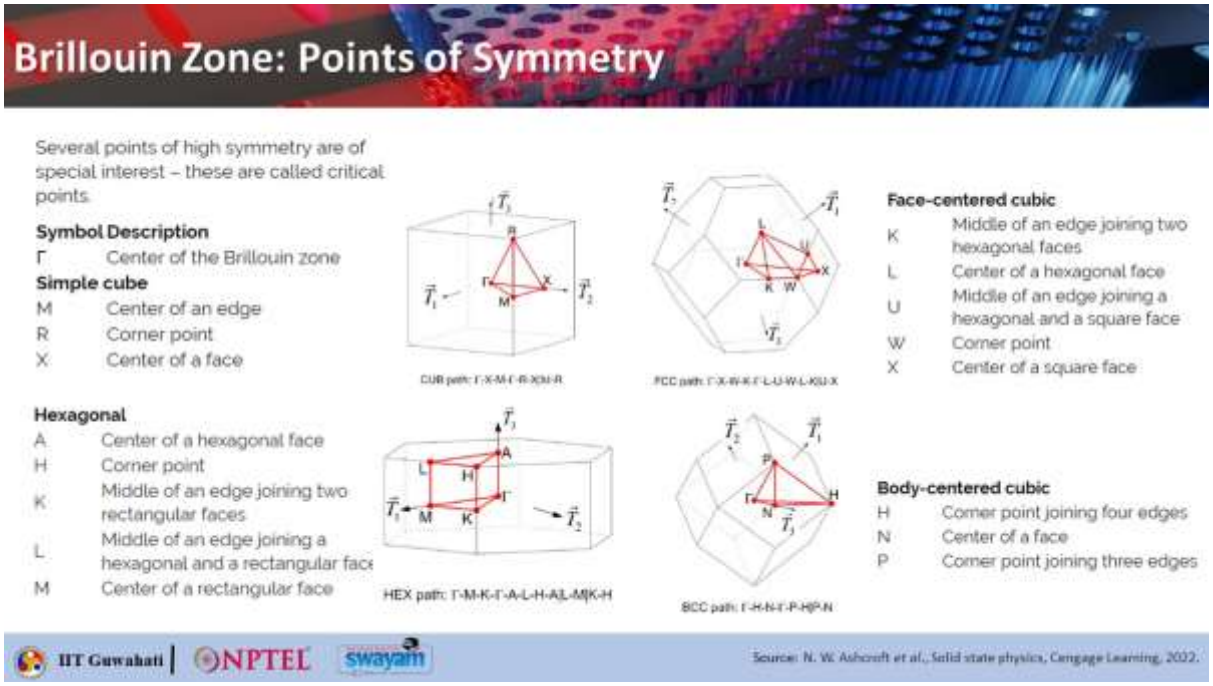


And finally, when you add up all the points, you will get, you know, this particular Wigner shade cell. Now, why it is important? If you think of Brillouin zone, which is very, very important for obtaining the properties of the photonic crystals to study the band structure and other properties.

So, Brillouin zone is basically constructed in the same way as the Wagner shell only difference is that Brillouin zone is constructed from the reciprocal lattice. So, Brillouin zone is closely related to the wave factors and diffraction. So, the analysis of periodic structures is is often done in the reciprocal lattice or reciprocal space. So, Brillouin zone for FCC lattice is basically a truncated octahedron with 14 sides ok or slide sides.



So, this is how it looks like ok. So, this is the Brillouin zone of a FCC. You can also draw this by yourself and try that. So, you can see that this is almost a spherical one and So, you can say that the FCC lattice has got the highest symmetry of the Bravais lattice. So, in terms of symmetry if you put this triclinic has got the lowest symmetry and then from simple cubic this is the Brillouin zone. then you have what is marked inside is the irreducible Brillouin zone okay. And then for BCC this is the Brillouin zone and this is the FCC Brillouin zone which you have seen.



Even for diamond you can get FCC Brillouin zone. So more or less you can see that the FCC one has got the highest symmetric Brillouin zone among the all Bravais lattice. And then if you go to pseudo periodic structure they have the highest symmetry in terms of the brilliant zone. So, now let us finally look into those irreducible brilliant zone and the important points of interest. So, several points of high symmetry are of special interest. So, if you think of a cubic lattice, so this is the cubic lattice brilliant zone, there gamma marks the center of the brilliant zone and then if you take m, m is basically the center of an edge, r is basically a corner point and x is basically the center of a face.

So, you can think of the three primitive reciprocal lattice vectors as t1, t2 and t3 and this particular volume here, that volume is the irreducible brilliant zone so how do you consider this as the path so you need to traverse along the boundaries of this irreducible brilliant zone to cover this entire volume. So, you can start with gamma, then you go to x, then to m, then to gamma. So, that covers the bottom part and then you go to r, okay. Then you come to x or m and then you come back to r, okay. So, that way you can actually then you again have gamma right so that will kind of complete traversing along the boundary points So if you consider hexagonal lattice, so this is the hexagonal lattice Brillouin zone.

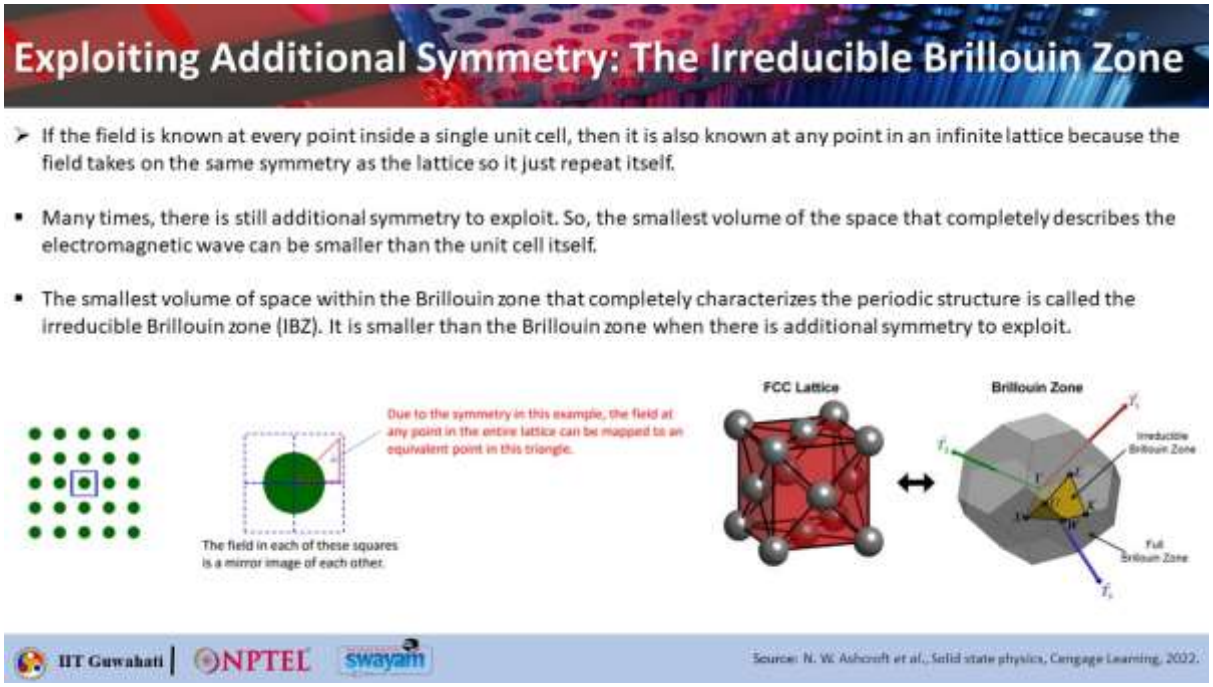
So here the important point is gamma is again the center of the Brillouin zone for each case. A tells you about the hexagonal center of hexagonal phase. H is basically a corner point. K marks the middle of an edge which joins two rectangular faces, means you are talking about this face and this face.

These are the two rectangular faces you are joining. So, this is K. L is marked as the, you know, middle of an edge which joins a hexagonal face with a rectangular face. So, this one is L and M is marked as a center of the rectangular face, okay. So, M here and M here do not actually designate the same points. So, you got to keep these things in mind.

So, these are the important points of symmetry depending on different lattice types. Similarly for FCC, You have K, L, U, W and X. These are the important points. And this is how the irreducible

brilliant zone looks like.

And for BCC, you have few points like H. H is the corner point joining four edges. n is the center of a face and p is basically corner point which is joining 3 edges and gamma is again the center. So, here you can mark capital T1, capital T2 and capital T3, these are the 3 primitive lattice vectors. And if you want to cover the BCC, the path will be gamma to h to n to gamma then to p then you can come back to H then n and then again gamma, but we do not repeat it correct. So, we this is the path for BCC. So why it is important to discuss about irreducible brilliant zone? Because if the field is known at every point inside a single unit cell, then it is also known at any point in the infinite lattice.



Because the field will just take on the symmetry of the lattice as the lattice is repeated. So many times what happened there is still additional symmetry to be explored. So only considering the unit cell itself is not enough. Sometimes there are symmetry within the unit cell that allows you to even focus on a smaller region where you can find some you know very independent modes okay and those modes can actually be you know those small region can be replicated few times to form your unit cell and then you can repeat your unit cell periodically. So that way it will bring down the computational requirement as well. So, the smallest volume of space within the Brillouin zone that completely characterizes the periodic structure is known as the irreducible Brillouin zone.

So, what we understood it is a much smaller area than the Brillouin zone itself where you have exploited additional symmetry. So, first this is the periodic lattice this is the square lattice and this blue marked area is basically the unit cell. So, ideally you should only study the property of this unit cell that will tell you about the property of this entire lattice. Now, within this unit cell you can see that you can actually mark the small triangular region okay where you can if you know the property of this triangular region you can take a you know rotational symmetry and get this particular quarter. You can have mirror symmetry you can form this upper half you can take another mirror symmetry and you can form the complete square.

right because the field in each of the square is a mirror image to each other right so using this concept you can reduce the amount of computation and you can only calculate the points or calculate the modes inside this irreducible brilliant zone So, what you understood that if you have taken FCCLAT is this is how the overall brilliant zone looks like, but this highlighted one is basically the irreducible brilliant zone and you can see for yourself that how small this volume is. So, the computation load is reduced, but you will be able to get the same information. Whatever properties you are seeing in this irreducible brilliant zone is the property there is nothing new outside it ok in the entire brilliant zone

So, with that we will stop here with this lecture on real and reciprocal lattices. If you have got any doubt you can always drop an email to me at this email address mentioning MOOC and photonic crystal on the subject line.