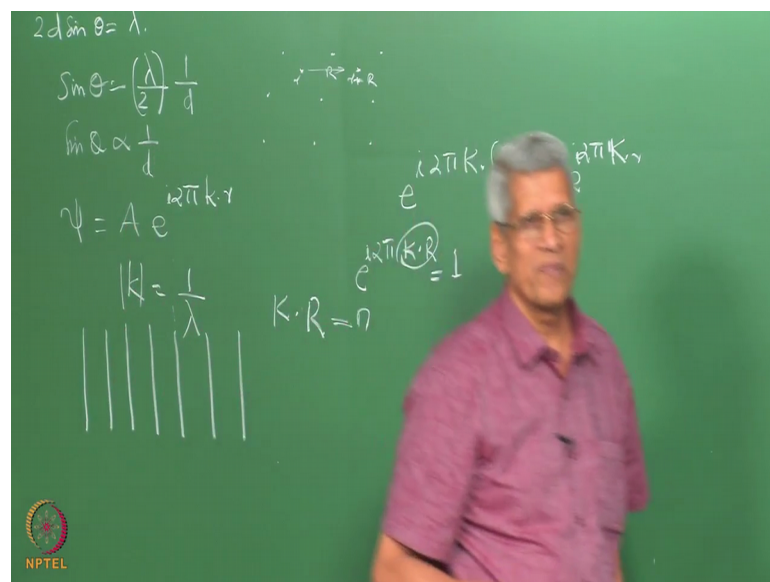


Electron Diffraction and Imaging
Prof. Sundararaman M
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

Lecture - 09
Reciprocal Lattice

Welcome you all to this course on Diffraction and Imaging. Today we will discuss about reciprocal lattice. So far in the last few classes we have discussed about how to use the information which is given in international unit of sonography to construct crystal structures correct? So, if you see here, we mention the lattice because generally this lattice is which is constructed for a Bravais Lattice.

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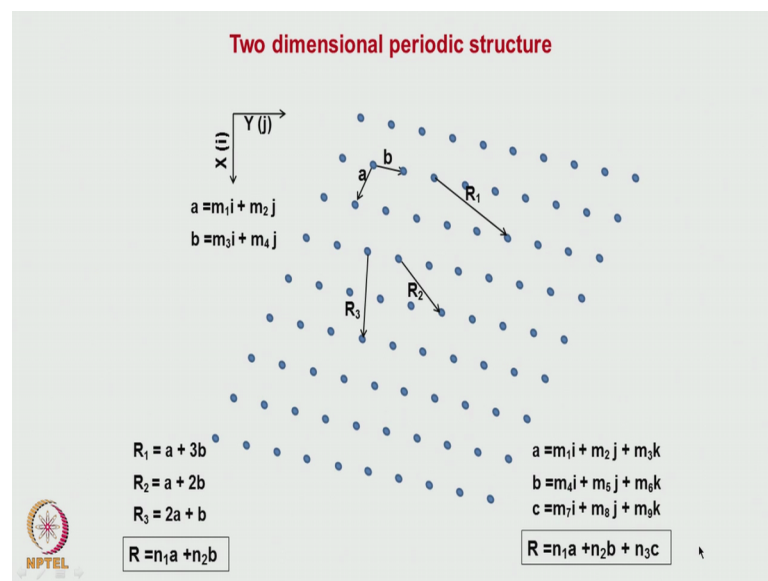
For a Bravais Lattice we construct a reciprocal lattice in the formula we use $2 d \sin \theta = \lambda$. λ is the wave length of the radiation which we use what is it which decides the crystal structure, what is the value at which you get the different peaks that corresponds to θ value or the $\sin \theta$ correct? So, this $\sin \theta$ will be nothing but $\lambda / 2$, you can take it this 2 , 1 by d correct? So, our $\sin \theta$ is proportional to 1 by d what is 1 by d , d is in real space correct? 1 by d is the reciprocal space. So, whether you like it or not every time you look at the diffraction pattern, either in TEM or in nutrient diffraction or in excide diffraction the information which you are getting it is

actually in reciprocal space right. So, that is one more other incentive to learn about the reciprocal lattice.

Then the other incentive is also is that when you look at the reciprocal the way we represent a periodicity. That is always we use a mathematical expression to represent it. So, even for an electromagnetic wave, when we represent it we write it as a to the power of $k \cdot r$, we represent it correct? This is how we represent an electromagnetic radiant or I should not call it as a wave because actually where we say misnomer essentially we call it as any periodic fluctuation. We will represent it in in this form what is k , k is nothing but 1 by λ .

So, again if you see the momentum space is nothing but an inverse of the real space, because of this whenever we do a diffraction experiment.

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If you have to derive a formula to find out how the scattering is taking place what is the way we represent the incident repro? Incident pro we represent it in terms of a expression like this. That is i is equal to $\exp(i k \cdot r)$ where the characteristic of the radiation is given by k which is in a reciprocal space. So, when these waves interact with that sample and the Bravais is getting scattered the scattered wave we also if we try to represent it, it is also represented in a reciprocal space. So, if you have to look at the interaction if we can represent the sample also in a reciprocal space it becomes much easier to do this calculation rather than trying to represent in a real space.

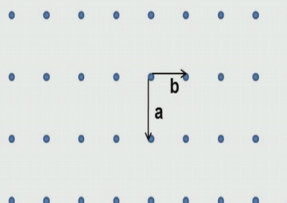
Here what I have done is just shown there are 2 dimensional periodic lattices. Here with respect to an orthonormal coordinate system, these vectors a and b can be represented in this particular fashion right. And then all these various vectors are nothing but what is going to be the translational periodicity in those directions in the lattice that is what it represents it is know this is for the 2 dimensional lattice which I had considered. 3 dimensional lattice we will be writing it an expression like this.

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Thought experiment

A field is filled with flag posts. It is assumed that they are arranged in a periodic way. An experiment has to be devised to find out whether periodicity exists and if so what is it?

A simple experiment can be conceived as follows: Arrangement of the flag post is as shown below with periodicity $\mathbf{R} = n_1\mathbf{a} + n_2\mathbf{b}$. Assume that a vehicle is moving at uniform velocity $\mathbf{v} = b/t$ parallel to the \mathbf{b} -axis with a camera mounted on top of a pole in the vehicle and the camera can rotate around the pole as the axis of rotation.



The diagram shows a 4x8 grid of blue dots representing flag posts. A vehicle, represented by a small rectangle, is moving horizontally between the second and third rows of dots. A camera, represented by a circle with a cross, is mounted on a pole on the vehicle. A vertical arrow labeled 'a' points downwards from the camera, and a horizontal arrow labeled 'b' points to the right. The NPTEL logo is in the bottom left corner.

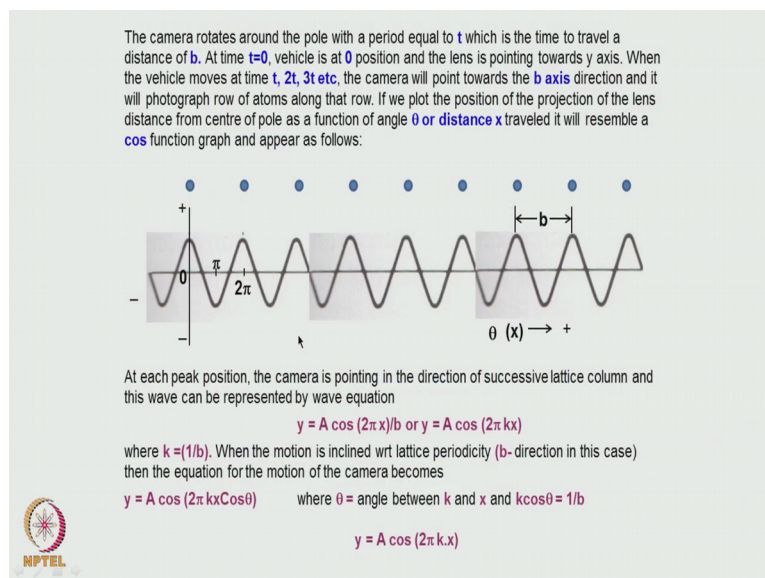
Now, let us look at this thought experiment. Suppose this is the position of atoms in a not atoms, we should call it as a lattice 2 dimensional lattice the position of the lattice points are given. It is a rectangular lattice this can be considered as like a real experiment, like suppose we have a lot of flag posts are being put for a republic differentiation. It is being arranged in a wave periodic way, but it is like a rectangular arrangement. Suppose I wanted to photograph this, but each row I wanted to take a photograph. So, what all the options which I have 2 directions means; 2 directions each row we have an to photograph alert to move across this row from here to here, and every time I will have to click when I am right. In front of this row correct? That is the one way in which we can do it.

I am considering an experiment where I am moving on a vehicle, in which on a pole I had fixed the camera. The camera can only rotate around the pole. And whenever if I can adjust the rotation of the camera around the pole in such a way that it moves from here to this position, where it reaches the camera faces all this row of atoms. When it goes from

here to here at a particular speed we will be able to capture all the rows will be taken with at a particular time it will be taken correct? If I try to plot a movement of the camera, how will it look like? How the camera has moved?

Student: (Refer Time: 06:50).

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With respect to distance this is the way it will come right. Because the camera is like this it moves like this it has to rotate around it, there is r and θ with which you can move the camera, but the camera is rotating around the axis, but this whole thing is moving right. If I try to plot it this is the sort of a periodic function with which we getting in. So, every time the camera reaches this particular across of this in this particular position, then you are going to (Refer Time: 07:24) going to click. So, this way I can get all the rows means missing out any of the atoms in this direction I can photograph it. Correct? Am I right? This is exactly what has been done.

So, if this wave has to be represented the way this camera, we have to represent it in formed of an expression. What is the sort of an expression which we will use, this is y is equal to $a \cos 2\pi x$ and if b is the distance between the wave an expression will come correct? So, every time camera reaches this particular one, it is clicking the photograph because all other layer atom positions are just behind it. Like this suppose instead of moving in parallel to this suppose we moving it in this direction, then what will happen? In that case the distance which I would be travelling here will be much more correct?


That means, that projection of this into this one has to be taken that projection if you try to take it that will nothing but a dot product correct? That is essentially what we write it as y equals $a \cos 2\pi$ correct? This way we can consider it.

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If \mathbf{k} and \mathbf{x} make an angle between them, then the function is $\mathbf{k} \cdot \mathbf{x}$. When the value of $\mathbf{k} \cdot \mathbf{x} = \pm n$ when n is an integer from 0 to ∞ , then the periodicity of the wave and the lattice is the same. Since $\mathbf{k} \cdot \mathbf{x}$ represents phase angle, it is a dimensionless quantity. $|\mathbf{k}| = \pm n/|\mathbf{x}|$. When $n=+1$, $|\mathbf{k}| = 1/|\mathbf{x}|$. The unit of \mathbf{k} is inverse of length. The $\mathbf{k} \cdot \mathbf{x} = \pm n$ means that product of \mathbf{x} and projection of \mathbf{k} in \mathbf{x} direction is an integer multiple.

ie., for every value of periodicity vector \mathbf{R} in the lattice, there exists plane wave with wave vector \mathbf{k} whose magnitude is inverse of \mathbf{R} . The set of wave vectors \mathbf{K} which satisfies this condition $\mathbf{K} \cdot \mathbf{R} = \pm n$ for all values of \mathbf{R} is called reciprocal lattice.

For every value of vector \mathbf{K} , there exist many values of \mathbf{R} which satisfy the condition, $\mathbf{K} \cdot \mathbf{R} = \pm n$ and these set of \mathbf{R} values represent direct lattice



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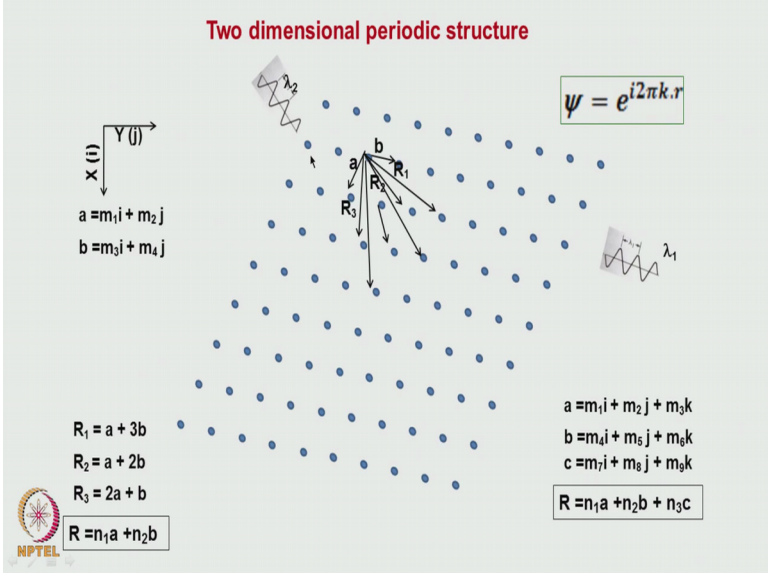
Two dimensional periodic structure

$\psi = e^{i2\pi \mathbf{k} \cdot \mathbf{r}}$

$\mathbf{a} = m_1 \mathbf{i} + m_2 \mathbf{j}$
 $\mathbf{b} = m_3 \mathbf{i} + m_4 \mathbf{j}$

$\mathbf{R}_1 = \mathbf{a} + 3\mathbf{b}$
 $\mathbf{R}_2 = \mathbf{a} + 2\mathbf{b}$
 $\mathbf{R}_3 = 2\mathbf{a} + \mathbf{b}$
 $\mathbf{R} = n_1 \mathbf{a} + n_2 \mathbf{b}$

$\mathbf{a} = m_1 \mathbf{i} + m_2 \mathbf{j} + m_3 \mathbf{k}$
 $\mathbf{b} = m_4 \mathbf{i} + m_5 \mathbf{j} + m_6 \mathbf{k}$
 $\mathbf{c} = m_7 \mathbf{i} + m_8 \mathbf{j} + m_9 \mathbf{k}$
 $\mathbf{R} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}$



Similarly, another experiment which we can think of is, suppose I am taking an electromagnetic radiation, had a plane wave pass allowing to pass through. So, the plane wave has it moves. It has crest and trough like this right. So, if we just mark this is how the crest is going to be, if that wave enters, as it moves if it has some wave length

λ . Then if I start with the crest touching on this atom position, as it moves in this direction there is no need that the crest should come out always there. What is the condition under which it will come?

For the particular value of λ where the value of k is equal to, if this is the translational vector in this direction is r_1 inverse of that correct? So, there is a specific value of λ at which it will occur right. This way by putting a wave like this, I can get all the atom positions that crest making fall; the same thing which I can do it in another direction. In this direction if I take bottle what should be the wave length of the radiation? It should be sum other value; so that has the wave passes through all the crest comes right on top of each of the lattice position.

Student: (Refer Time: 10:32).

In that direction that is $1/r$ will be the- so in that one that is the way the expression will turn out to be. Otherwise in the that direct lattice, if we see that when the crest from one to the other it will be the distance here in this case r_2 , but when we are express it as a wave the property of the how we mathematically express it, it is only the k which represents the way and a represent the scattering from the interaction the strength of the radiation correct? These are all the 2 factors which define the radiation (Refer Time: 11:11) exactly that same thing is what we are doing it here also.

So, if you do this now how do we represent it? Suppose I choose some particular point here like here, I mark a point here. From this point which is the point at which an identical position will come if we are moving in this direction may be from somewhere here right.

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$$\psi = e^{i2\pi k \cdot r}$$

Incident plane wave


If R represents set of points representing Bravais lattice and ψ represent plane wave, then for any general k plane wave will not have periodicity of Bravais lattice. The set of wave vectors K for which plane wave will have the periodicity of lattice is known as reciprocal lattice. Then

$$e^{i2\pi K \cdot (r+R)} = e^{i2\pi K \cdot r}$$

The reciprocal lattice as a set of wave vectors K satisfying the equations

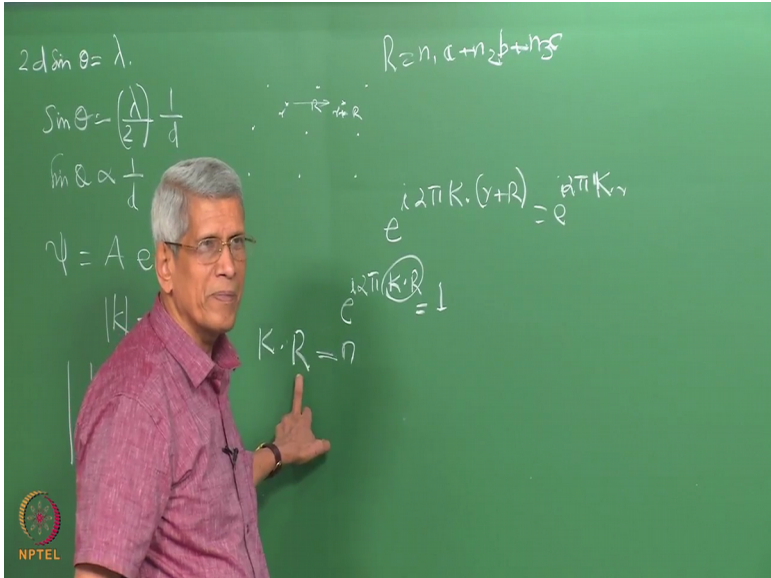
$$e^{i2\pi K \cdot R} = 1$$

for all R in the Bravais lattice.




How will we represent these 2 points will be representing it as e to the power of $i2\pi$. Now k I am choosing it as a specific value, because that is the value with which we are choosing the radiation. Then $k \cdot 1$ is r plus r right from an origin which we have chosen.

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The chalkboard contains the following derivations:

- $2d \sin \theta = \lambda$
- $\sin \theta = \left(\frac{\lambda}{2}\right) \frac{1}{d}$
- $m \lambda \propto \frac{1}{d}$
- $\psi = A e^{i2\pi k \cdot r}$
- $R = n_1 a + n_2 b + n_3 c$
- $e^{i2\pi K \cdot (r+R)} = e^{i2\pi K \cdot r}$
- $e^{i2\pi K \cdot R} = 1$
- $K \cdot R = n$



This point is at r and another this point is r plus r . Because this distance is a vector r , then the expression turns out to be should be equal to e to the power of $i2\pi k \cdot r$; this what it will turn out to be.

So, this will finally lead to a condition $k \cdot r$ should be equal to 1 correct? So, this is one of the most significant expressions, which we have to consider as far as a reciprocal lattice is concerned. So, if this value has to become one what should be the value of $k \cdot r$ this vector.

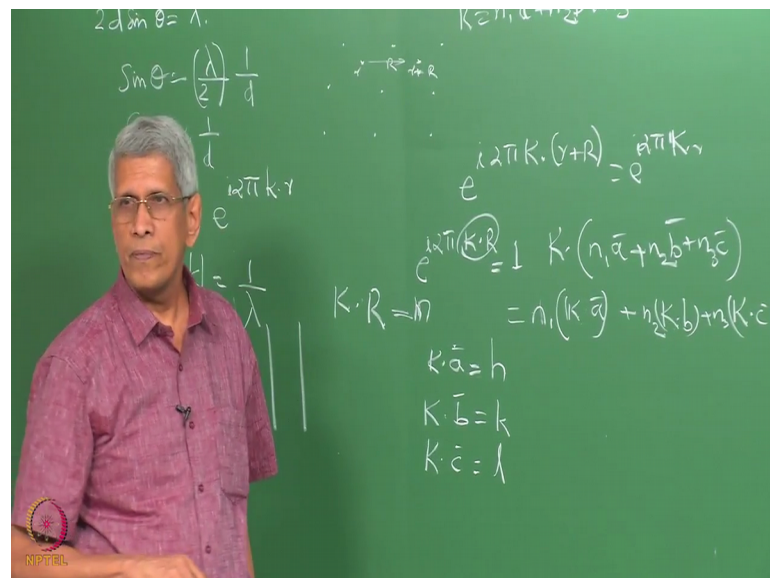
Student: (Refer Time: 13:18).

What not 0m it can be any integer including 0.

Student: (Refer Time: 13:30).

It can be passed in a it any value it can change right. These are value which is possible, correct? So, then for all those values that is, if we take this here a dot r equals to 1 also this will be one na $k \cdot r$ all are 0 also will be one minus also and also it is it does not matter what the value is, but this has to be an integer. This is clear? Now suppose we are considering this with respect to particular some specific r value we choose it here. Generally how do we represent the direction in a lattice? n_1 into a plus n_2 into b plus n_3 into c this is the way we can write it right.

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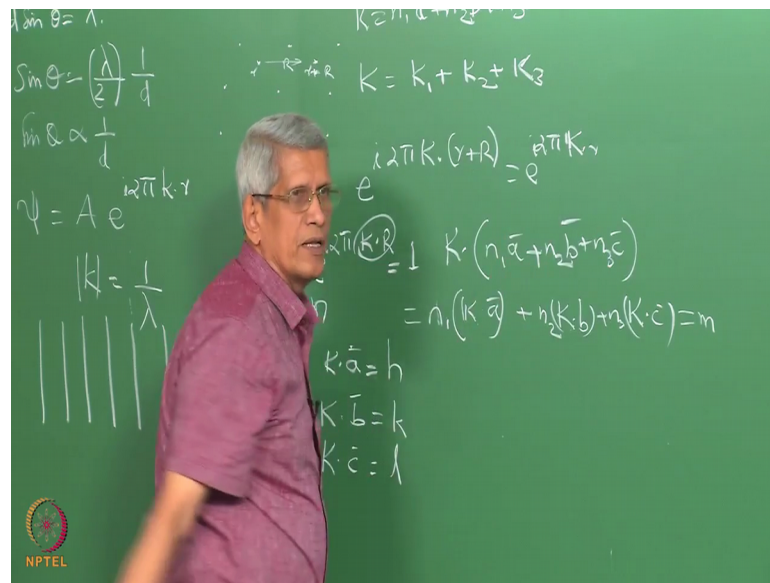


If I substitute it here, then what this expression will become? That is $k \cdot r$ this should become n_1 , n_2 $k \cdot a$ plus n_2 into $k \cdot b$ plus n_3 into $k \cdot c$, correct? And this has to become suppose I write it as a constant m , if this value m has to be an integer it has to be an integer for all values, all independent values; that means, that since n_1 n_2 n_3 is an

integer in the lattice, this 3 terms have to be an integer independent each one of them individually has to become an integer. So; that means, that $\mathbf{k} \cdot \mathbf{a}$ I just write it as an integer h $\mathbf{k} \cdot \mathbf{b}$ $\mathbf{k} \cdot \mathbf{c}$ is equal to l .

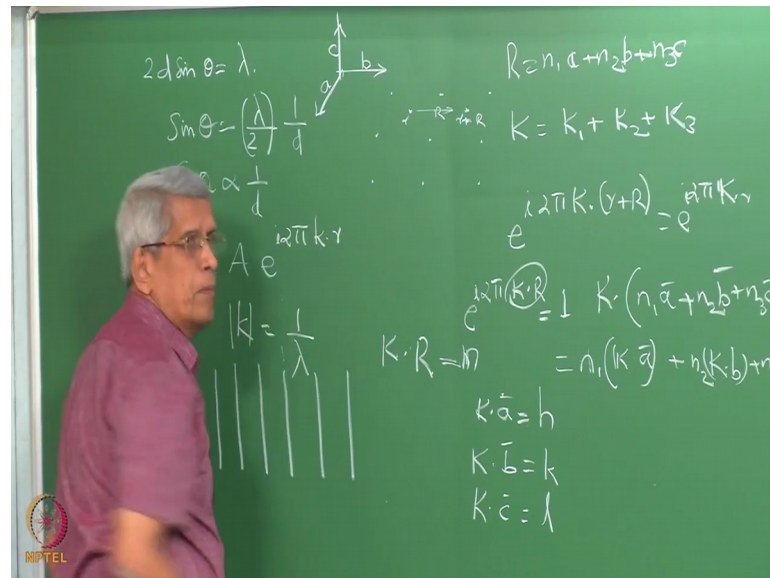
This way we can write in some integer, we did not know what the value is. So, our aim is to find out now what should be the value of \mathbf{k} correct? That is what we have to derive, because this \mathbf{k} is some vector in the reciprocal space. How does it relate it to the real space that information we have to get it? What we can do it is that \mathbf{k} since it is a vector.

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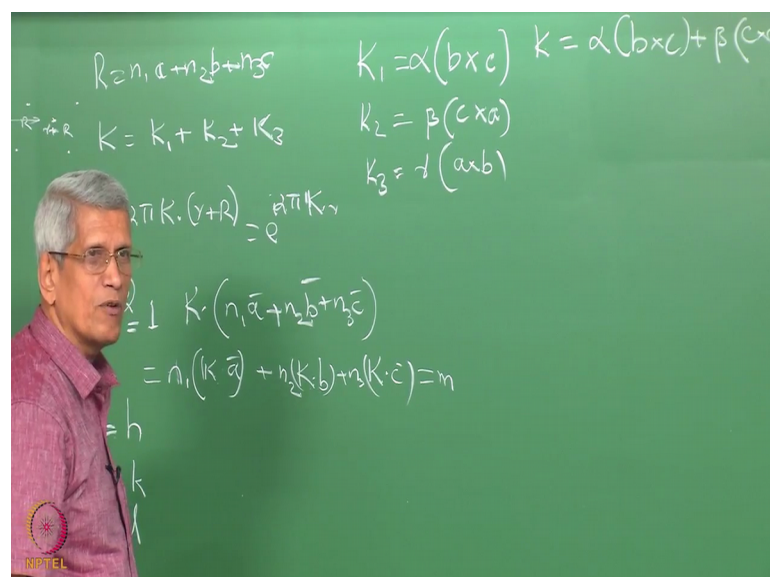
We can write \mathbf{k} as equal to k_1 plus k_2 plus k_3 these are all the components into this one a modulus of k_1 in to it turn out to be right. The x y and z direction this way we can write it.

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Suppose we wanted to find out what $k_1 k_2 k_3$ is, since we know the axis which we have chosen here or suppose we write like this. And this is a and this is b and this is the c axis of the crystal, whatever you have chosen in itself, then the $b c$ plane is going to be the one which is in the a axis direction correct? Is it not? If I take a vector product of b cross c , what does it denote a vector normal to that plane $b c$ plane that is vector normal to the $0 0 1$ plane it gives it.

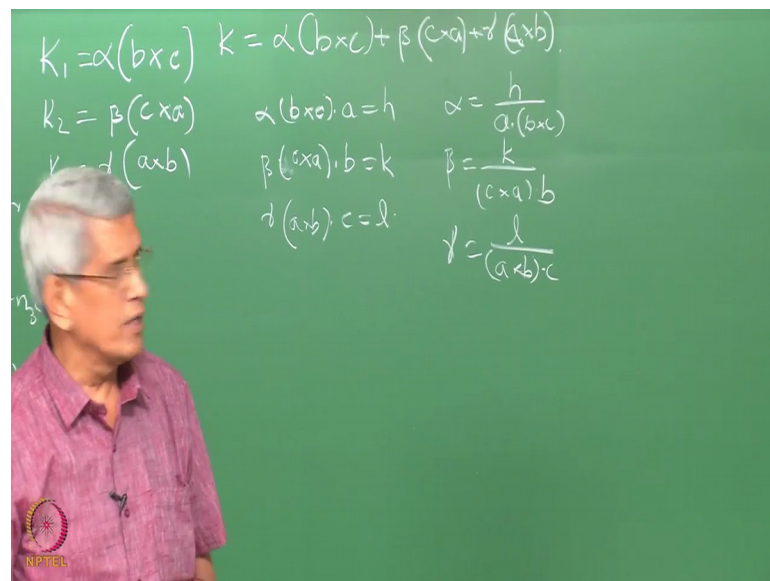
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So, that will turn out to be that is I can write k to be equal to sum constant into b cross c , what we do not know the value of α or γ .

Similarly, k can be written as β into c cross a k can be written as γ into a cross b . We are doing this exercise to find out what is the relationship between reciprocal and real space this is.

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The chalkboard contains the following derivations:

$$k = \alpha(b \times c) + \beta(c \times a) + \gamma(a \times b)$$

$$k_1 = \alpha(b \times c) \quad k_2 = \beta(c \times a) \quad k_3 = \gamma(a \times b)$$

$$\alpha(b \times c) \cdot a = h \quad \alpha = \frac{h}{a \cdot (b \times c)}$$

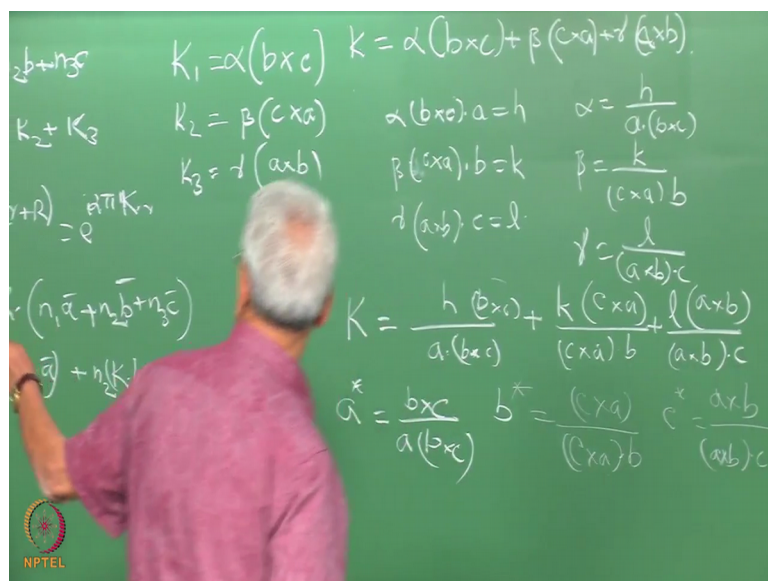
$$\beta(c \times a) \cdot b = k \quad \beta = \frac{k}{(c \times a) \cdot b}$$

$$\gamma(a \times b) \cdot c = l \quad \gamma = \frac{l}{(a \times b) \cdot c}$$

So, now this vector if we write, this vector k will be in to a cross b correct? Now if we, if I substitute this k in here, now what it will turn out to be if I take the dot product with respect to this k , it will be α into b cross c dot a will turn out to be h . Correct? This is the sort of an expression; we will get it β will be β into c cross a dot b will be equal to k γ into a cross b dot c will be equal to l .

From this we have got α β all these expressions which we have got the value of α equals h by a dot b cross c right. β equals k by c cross a dot b γ equals l by right. These expressions are right. So, this is what if you substitute this into this expression for k .

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The chalkboard contains the following equations and derivations:

$$K_1 = \alpha(b \times c) \quad K = \alpha(b \times c) + \beta(c \times a) + \gamma(a \times b)$$

$$K_2 = \beta(c \times a) \quad \alpha(b \times c) \cdot a = h \quad \alpha = \frac{h}{a \cdot (b \times c)}$$

$$K_3 = \gamma(a \times b) \quad \beta(c \times a) \cdot b = k \quad \beta = \frac{k}{(c \times a) \cdot b}$$

$$\gamma = \frac{l}{(a \times b) \cdot c}$$

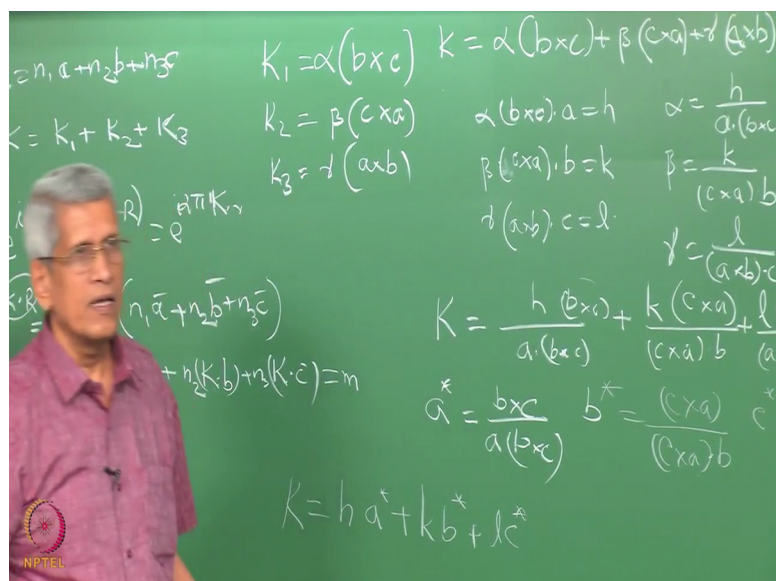
$$K = \frac{h}{a \cdot (b \times c)} + \frac{k}{(c \times a) \cdot b} + \frac{l}{(a \times b) \cdot c}$$

$$a^* = \frac{b \times c}{a \cdot (b \times c)} \quad b^* = \frac{(c \times a)}{(c \times a) \cdot b} \quad c^* = \frac{a \times b}{(a \times b) \cdot c}$$

Now, what it becomes k becomes h by a dot b cross c right, into b cross c k into c cross a by c cross b , l into a cross b a cross b dot c correct? Is it not? If i, because what this value are is only nothing but the alpha value which you have founded the magnitude now. So, this is we can take it as k a k b k c, or we can write it as this itself can be written as if I write it as a star b cross c , correct?

Similarly, I am just denoting it this way. So, using this simple relationship, that k dot r has to be an integer right. We have just derived an expression for what is the relationship between k we have derived right. And the k is nothing but it will be h into a star plus k into b star plus l into c star.

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The chalkboard contains the following equations:

$$\mathbf{r} = n_1 \mathbf{a} + n_2 \mathbf{b} + n_3 \mathbf{c}$$

$$\mathbf{K} = \mathbf{K}_1 + \mathbf{K}_2 + \mathbf{K}_3$$

$$\mathbf{K}_1 = \alpha (\mathbf{b} \times \mathbf{c}) \quad \mathbf{K} = \alpha (\mathbf{b} \times \mathbf{c}) + \beta (\mathbf{c} \times \mathbf{a}) + \gamma (\mathbf{a} \times \mathbf{b})$$

$$\mathbf{K}_2 = \beta (\mathbf{c} \times \mathbf{a}) \quad \alpha (\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a} = h \quad \alpha = \frac{h}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}$$

$$\mathbf{K}_3 = \gamma (\mathbf{a} \times \mathbf{b}) \quad \beta (\mathbf{c} \times \mathbf{a}) \cdot \mathbf{b} = k \quad \beta = \frac{k}{(\mathbf{c} \times \mathbf{a}) \cdot \mathbf{b}}$$

$$\gamma (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} = l \quad \gamma = \frac{l}{(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}}$$

$$\mathbf{K} = \frac{h (\mathbf{b} \times \mathbf{c})}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} + \frac{k (\mathbf{c} \times \mathbf{a})}{(\mathbf{c} \times \mathbf{a}) \cdot \mathbf{b}} + \frac{l (\mathbf{a} \times \mathbf{b})}{(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}}$$

$$\mathbf{a}^* = \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \quad \mathbf{b}^* = \frac{\mathbf{c} \times \mathbf{a}}{(\mathbf{c} \times \mathbf{a}) \cdot \mathbf{b}} \quad \mathbf{c}^* = \frac{\mathbf{a} \times \mathbf{b}}{(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c}}$$

$$\mathbf{K} = h \mathbf{a}^* + k \mathbf{b}^* + l \mathbf{c}^*$$

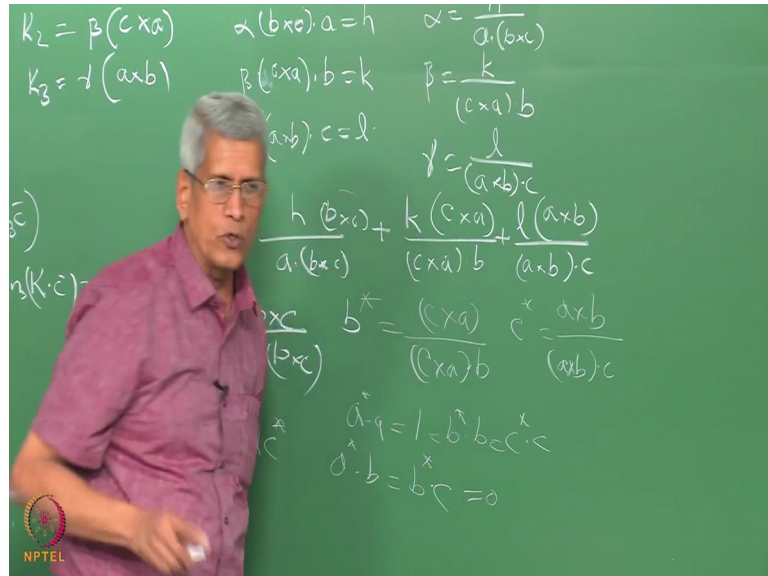
This is a vector in the reciprocal lattice correct? h, k, l are the coefficients of that vector right. If you look at this vector the definition, it is essentially with an orthonormal axis both the coordinates systems are the same coordinates system with which all the vectors are derived right. Represented is this clear?

So, naturally that is for every vector you can have a reciprocal vector. This is actually in vector algebra is called as a dual space. Therefore, for every space in a vector there is a reciprocal space which is always going to exist that is apart from this. So, now, what you can make out is in if the vectors in the real lattice exhibit whatever is the symmetry, the same symmetry will be exhibited by the lattice which is generated by using this vectors. So, the reciprocal lattice and the real lattice exhibit all the symmetry of that crystal structures, but one is expressed in a real lattice, but the same symmetry everything is exhibited by, So, what does it mean that is when we put a sample which exhibits some symmetry. The experimental information which we collect it also exhibits the complete symmetry, but it is expressed in a reciprocal space correct? The information comes in that space it exhibits it.

So, you see analyze and get information about what we get it in the reciprocal space we can immediately find out information about that crystal structure into real space. That is what the game is, but it is easier said than that. So, there are so many people have done it

millions of scientist on various aspects of it that I think possibly some of you also may be working on this in future. What is the other property of it?

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The consequences of it is that, a star dot a will be equal to 1 equal to b star dot b, equal to c star dot c correct? Similarly, a star dot b, equals b star dot c these are all will be equal to 0; these expressions having got this expression. Now you can substitute and just check all these expression that I will leave it as a problem for you to work out, and then you will understand how it will come. Then another one is the yes venkatesh.

Student: Second condition a star dot b and a star dot.

C.

Student: Is it 0.

It actually.

Student: It begins with real lattice as orthonormal.

No.

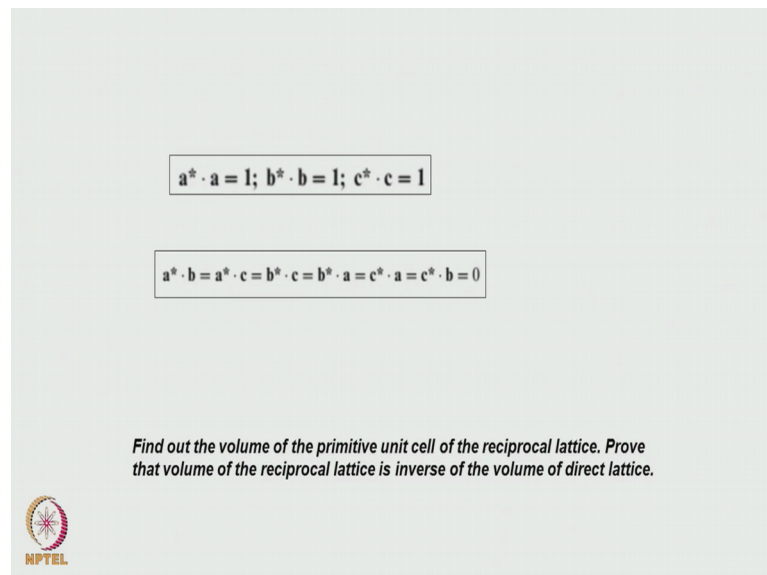
Student: Perpendicular.

No need not.

Student: A b c.

A b c need not can be any value. It is an orthonormal system in which we are representing these vectors a b and c. But the vector algebra if you choose any vector a and b to define it that the all the expressions whatever we derived all are valid. And what we do it is that, one thing one should remember is that we have used here the shortest translational vectors are essentially a primitive lattice which we have considered. Reciprocal lattice is constructed for the primitive lattice of the structure that is how it is always derived.


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$$\mathbf{a}^* \cdot \mathbf{a} = 1; \mathbf{b}^* \cdot \mathbf{b} = 1; \mathbf{c}^* \cdot \mathbf{c} = 1$$

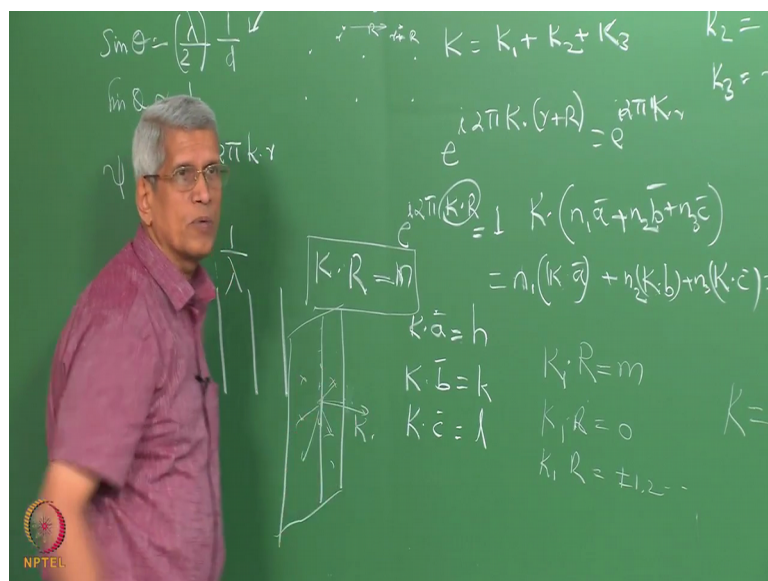
$$\mathbf{a}^* \cdot \mathbf{b} = \mathbf{a}^* \cdot \mathbf{c} = \mathbf{b}^* \cdot \mathbf{c} = \mathbf{b}^* \cdot \mathbf{a} = \mathbf{c}^* \cdot \mathbf{a} = \mathbf{c}^* \cdot \mathbf{b} = 0$$

Find out the volume of the primitive unit cell of the reciprocal lattice. Prove that volume of the reciprocal lattice is inverse of the volume of direct lattice.



So, this expression, see it is something like this is what is a star? A star contains a term b cross c right. B star that is b cross c if you take it, and that vector it will be always perpendicular correct? So, that is what will happen to a dot product if you take with respect to be they are perpendicular to each other. So, that is 0 that is what essentially it means. This has nothing to do with that coordinate system. Now what does this mean? If this $\mathbf{k} \cdot \mathbf{r}$ equals m, here again I come back to in because one should fully understand what the significant of this that equals m means, that if I choose a particular vector in the real lattice \mathbf{r} , there can be many values of \mathbf{k} for which this equation will be satisfied. Or suppose I choose a specific value of \mathbf{k} .

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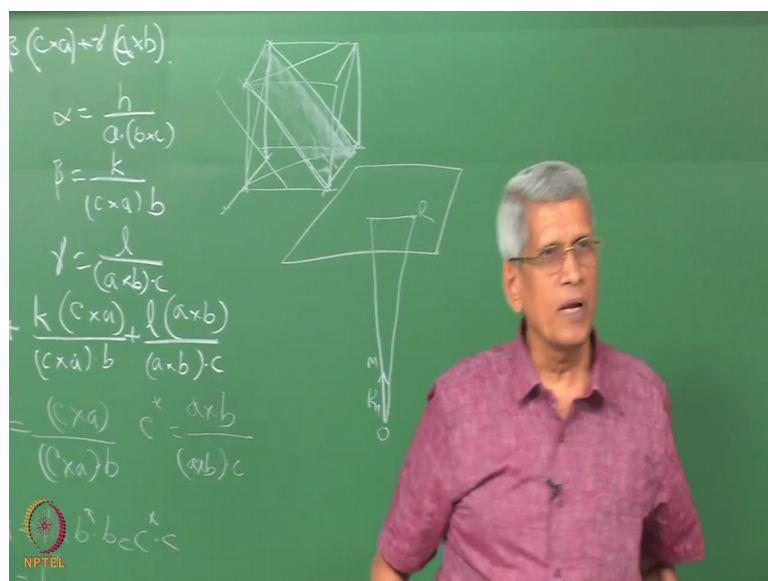


Some particular vector I choose it to be k_1 that $k_1 \cdot r$ equals m I take it right. What all we can $k_1 \cdot r$ could be equal to 0, $k_1 \cdot r$ could be equal to plus minus any number 1 2 like that it can happen is it not, k_1 to mean so many values of r which we can choose it.

Let us just take that case $k_1 \cdot r$ equals 0. What does it mean? For a particular value of k_1 which has been chosen what is k_1 , k_1 is normal to a particular plane right. Plane normal, but that vector with the magnitude which is inverse of the inter particles spacing between those planes right. So, if we take a plane like this, and suppose this is k_1 , k then there can be many atoms in this plane should be there no, with vectors from here to here if I consider this as a plane which comes likes this.

And this is what the vector k_1 needs. So, there can be many positions, periodic position should be there this are all, if this is the origin with $r_1 r_2 r_3$ like this. So, many vectors are there all these vectors are perpendicular to that k_1 , k_1 is only one vector in reciprocal space to that vector there are many periodic distances are there. So, when $k_1 \cdot r$ equals 0, means that all that values of r which represent is a plane which passes through the origin and which is perpendicular to k_1 , that is the plane which it represents.

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Like for example, suppose I take a simple cubic lattice. I can have a plane which is like this is 1 1 1 plane right. There can be an 1 1 1 plane that can be like this. 1 1 1 plane can pass through this another 1 1 1 plane can pass through this origin also. That particular condition also represents the plane which is passing through the origin, is it clear? What does $k \cdot r = 1$ represent.

Student: (Refer Time: 30:25).

It will represent the plane which is parallel to it nearest to it. All the atoms in that plane are the once we satisfy that condition, for the same $k \cdot r = 1$ right. Similarly $k \cdot r = 2$ will represent the third plane like this. So, like that now if you will look at it, almost all the lattice planes which are in that particular direction sitting one on top of the other. If we represent that by a vector the lattice translational vector with respect to the origin, that dot product if we take it with respect to the reciprocal or particular reciprocal lattice vector that is satisfies this equation.

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Meaning of $\mathbf{K} \cdot \mathbf{R} = n$ where N is an integer

The reciprocal lattice is defined by a set of wave vectors \mathbf{K} for which

$$\exp(i2\pi\mathbf{K} \cdot \mathbf{R}) = 1 \text{ ----- (1)}$$

where \mathbf{R} represent lattice translation vectors in the Bravais lattice. For this condition to be satisfied $\mathbf{K} \cdot \mathbf{R} = n$ where n is an integer from $-\infty$ to $+\infty$ including zero. For all these values of n , the value of RHS in equation (1) becomes 1.

(It should be noted that for this condition, the amplitude of the waves scattered from all lattice points in the direction of \mathbf{k}' add together giving rise to maximum amplitude or constructive diffraction condition)

Let us consider the case $\mathbf{K} \cdot \mathbf{R} = 0$

For a dot product to be zero, the vectors \mathbf{K} and \mathbf{R} should be perpendicular to each other. This means for a specific value of \mathbf{K} say \mathbf{K}_1 , there exist many \mathbf{R} vectors in the direct lattice for which $\mathbf{K}_1 \cdot \mathbf{R} = 0$. All \mathbf{R} vectors \perp to \mathbf{K}_1 lie in a plane. This condition is satisfied for lattice point at origin also, for which $\mathbf{R} = 0$. In short this condition represents a plane passing through the origin and \perp to \mathbf{K}_1 .

Alternate interpretation: $\mathbf{K}_1 \cdot \mathbf{R} = 0$ means $K_1 R \cos\theta = 0$ where θ is the angle between \mathbf{K}_1 and \mathbf{R} and for this condition, $\theta = 90^\circ$ $\cos\theta = 0$. Hence \mathbf{K} and \mathbf{R} normally have non zero values.)

So, though entire lattice points have been covered now it is not. So, this expression this is equivalent to any doubt. So, this is equivalent to suppose I have a take a plane like this. This is a point r , in the real space. And this is from here I take it suppose this o m is going to be that k_1 . If I take this $r \cdot k_1 \cdot \cos \theta$ will represent some value n . That is essentially nothing but projection of it into this one. If that turns out to be an integer also this satisfies that. So, essentially on various planes we can have atoms which are there all of them can satisfy this equation yes.

Student: Sir, there when you were explaining 1 1 1 planes actually that is not passing from origin. So, how we can?

Like this what I can do it is that instead of taking a this plane, I can take a plane which may be inclined like this. This plane also is a plane which is there. There can be another plane which passes through this there can be a plane which passes through the origin like that. So, many planes will be there no with respect that will correspond to another k_1 value k value. In that way also if we consider it for that specific value of k_1 almost all the atoms which are there on various planes they will satisfy this condition. So, this is the condition which has to be satisfied between the real lattice and the reciprocal lattice. You understand that? So, what this meaning of each of this expression means is nothing but with respect to a particular reciprocal lattice which vector which we have chosen. All the

other vectors which are going to be there on different planes in the real lattice they satisfy this condition $\mathbf{k} \cdot \mathbf{r} = m$ which is an integer.

Is it clear? These are most significant aspect of the reciprocal lattice.

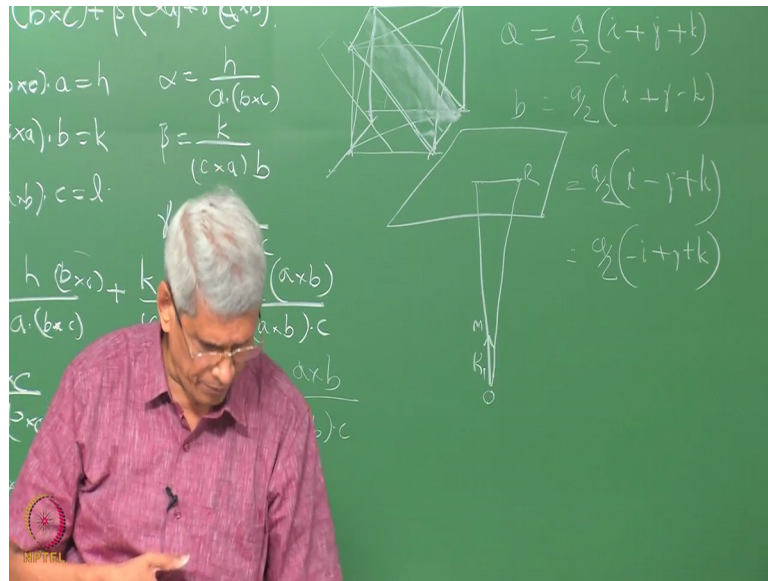
Student: Sir, here origin same for both.

Origin is the same with respect to same origin that is why we are choosing a orthonormal axis system, with which initially when we started we are choosing with respect to this an orthonormal with using this coordinate system, we are defining \mathbf{a} and \mathbf{b} right. Similarly, \mathbf{a}^* and \mathbf{b}^* also when we define it is defined with respect to a same coordinate system. Only thing what happens is that the coefficient of them of these vector are this lattice translational vectors will be one is inverse of the other you understand that. So, what we have tried to do is just try to find out what is the meaning for this \mathbf{k} vectors under what condition we can generate our reciprocal lattice.

So, using these expressions, we can derive generate a reciprocal lattice for a real lattice given a lattice parameters \mathbf{a} , \mathbf{b} and \mathbf{c} . This there are many conditions which we can that is this same reciprocal lattice, suppose it is going to be a triclinic lattice. If it is going to be a tetragonal lattice, all of them I think I will make you do a some exercise. So, that you understand how the reciprocal lattice comes. So, essentially what one has to do is if the lattices is the primitive lattice, like simple cubic system is a primitive one we know where the \mathbf{a} , \mathbf{b} and \mathbf{c} parameters are known.

Now, suppose we take a body centered lattice. Then what we have to do? We have to first find out the primitive lattice vectors. That primitive lattice vectors in the last classes.

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In the regular this one we have seen that it will be like one vector could be it will be a by 2 one is i plus j plus k right. The vectors another will be i plus j minus k. There are 4 vectors will come off this one we will choose 3 of them to define that coordinate coordinates. And now when we know this vectors a b and c, this is a this is b and c if you know then using this expression, we can find out the reciprocal lattice vectors. Then we can try a unit cell corresponding to that. That is what we find that when you try to create a unit cell in reciprocal space for a BCC unit cell.

Student: FCC.

Right, FCC and FCC unit cells resembles like.

Student: BCC.

BCC correct; simple cubic will look like so, but for others there will be some rotational also will be there. That is why I would like you people to do some assignments looking at non cubic systems. Then you will understand this reciprocal lattice concept, how to do it. This is one to construct it and then another is that we since we know the planes which we are taking it, the vector which is perpendicular to that. With respect to that now we can index each reciprocal lattice vector represents a particular plane in the lattice, correct? So, that point if a plane we index it as h k l, then the reciprocal lattice point also we can index it as h k l right. That is the way we can represent it. And since we are

choosing a primitive lattice, what is the advantage of using a primitive lattice? That is when you look at the extension condition which will come to later, is that none of the points are missed because all lattice points are scanned here.

Naturally it takes care of the extension condition, when you construct a reciprocal lattice. If this will come to now itself, what we will do it is that this is a mathematical expression way in which we have to try a reciprocal lattice, we have looked at it correct? That is b that is another vector could be a by 2, i minus j plus k a by 2, minus i plus j plus k these are all nothing but 3 vectors which are 1 1 1 vectors which we are taking in it that generates the rhombohedra lattice correct? We will come back to it later.

Suppose we have to construct this what is the geometrical way in which we can construct a reciprocal lattice. This is the same mathematical operation we can do it also. Mathematical way is that most elegant way of looking at it.

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Let us consider the case $\mathbf{K}_1 \cdot \mathbf{R} = 1$

This means $\mathbf{K}_1 \cdot \mathbf{R} \cos\theta = 1$ ----- (2)


or $\cos\theta = \frac{1}{\mathbf{K}_1 \cdot \mathbf{R}}$. This condition is satisfied for all those \mathbf{R} vectors for which the product of its projection with \mathbf{K}_1 is equal to 1 ($\mathbf{R} \cos\theta = \text{a constant}$). This set of \mathbf{R} vectors defines another plane parallel to the one passing through the origin and this is adjacent to the one passing through origin. The smallest value of \mathbf{R} in this case is when $\cos\theta = 1$ or \mathbf{K}_1 and \mathbf{R} are parallel to each other. In this case, $|\mathbf{R}| = 1/|\mathbf{K}_1|$ and this distance corresponds to the interplanar spacing. It is possible that there is no lattice point (lattice vector) is present in this plane which is parallel to \mathbf{K}_1 .

Following this argument, one can say, all \mathbf{R} vectors that satisfy the condition $\mathbf{K}_1 \cdot \mathbf{R} = 2$, lie in a plane next to first plane.

From the above discussion, it is clear that for every value of $\mathbf{K}_1 \cdot \mathbf{R} = 1, 2, 3, \dots$ one can find a set of values of lattice translation vectors, \mathbf{R} satisfying this condition and lying in a plane and these planes are parallel to each other.

When for all possible values of n for equation (1) is considered for a specific value of \mathbf{K}_1 , the entire lattice points are taken into account.

It can so happen that for a specific value of $n = N$, there exist a lattice translation vector \mathbf{R} lying in the plane for which is $\mathbf{K}_1 \cdot \mathbf{R} = N$ and $|\mathbf{R}| = (N/|\mathbf{K}_1|)$. The magnitude of this vector \mathbf{R} is the shortest distance between origin and the plane satisfying the condition $\mathbf{K}_1 \cdot \mathbf{R} = N$. This vector \mathbf{R} decides the periodicity of the lattice in the direction \mathbf{R} . Between this vector and the origin, there exists N planes which are parallel to this plane and perpendicular to reciprocal lattice vector \mathbf{K}_1 .




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The reciprocal law

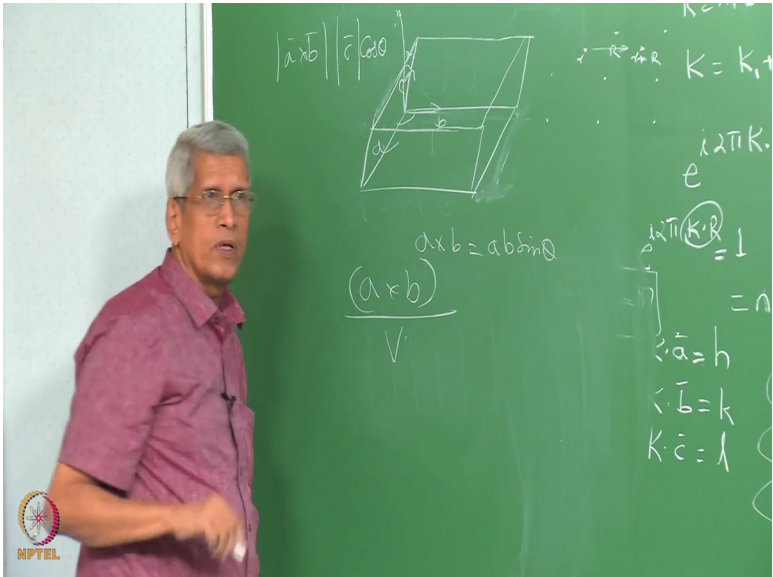
To each set of direct lattice planes corresponds a reciprocal lattice vector

To each set of reciprocal lattice planes corresponds a direct or real lattice vector



This is what the law which is called as the reciprocal law, that is for every set of direct lattice planes, corresponds to each set of a direct lattice planes corresponds to a reciprocal vector that is vector, similarly for each set of a reciprocal lattice set of reciprocal lattice planes they correspond to one direct vector. That is what that is all different way of interpreting the same expression $\mathbf{k} \cdot \mathbf{r}$ should be equal to an integer. What does this essentially mean? All these expressions which we have taken are here.

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$\mathbf{a} \times \mathbf{b} = ab \sin \theta$

$\frac{(\mathbf{a} \times \mathbf{b})}{V}$

$\mathbf{K} = \mathbf{K}_1 + \mathbf{K}_2$


$e^{i2\pi \mathbf{K} \cdot \mathbf{r}}$

$e^{i2\pi (\mathbf{K} \cdot \mathbf{R})} = 1$

$\mathbf{K} \cdot \mathbf{a} = h$

$\mathbf{K} \cdot \mathbf{b} = k$

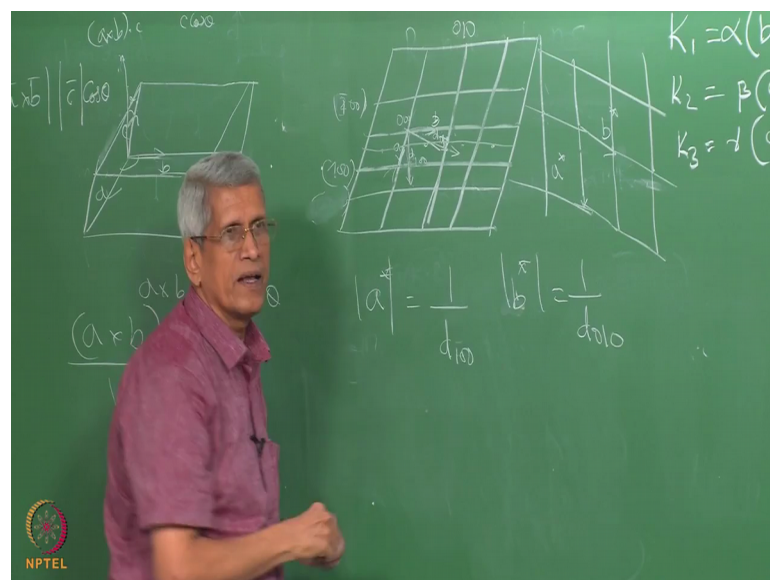
$\mathbf{K} \cdot \mathbf{c} = l$



$\mathbf{b} \times \mathbf{c}$ by this can be considered like; suppose we take I do not know whether I had drawn it correctly or not; it is a \mathbf{b} and \mathbf{c} what does a $\mathbf{b} \times \mathbf{c}$ means? It is a \mathbf{b} the angle between them $\sin \theta$ correct; physically that what it means, that we consider in a vector algebra is a vector which is perpendicular to it. Actually what that magnitude is nothing but area of this parallelogram correct? And what is and that is what we define it as a vector in this direction a $\mathbf{b} \times \mathbf{c}$ correct? What does this dot \mathbf{c} means that, it is nothing but projection of \mathbf{c} onto a $\mathbf{b} \times \mathbf{c}$ the projection of \mathbf{c} will be nothing but $c \cos \theta$ if this angle is θ $c \cos \theta$ correct. This $c \cos \theta$ angle is nothing but the perpendicular distance between the planes; is it not $c \cos \theta$ is nothing but the perpendicular distance between the 2 planes which we are considering it.

That is the area multiplying with the perpendicular distance vector algebra. If you take this vector $\mathbf{a} \times \mathbf{b}$, divided by the volume is what are we doing area divided by volume you put it is nothing but inverse of the height, but the direction is the same. So, it is in the direction which is perpendicular to that vector whatever the planes which are there that height which we are taking correct? Is it not this is exactly what is being d_{100} by all this vector algebra operation the same thing we can do it on any crystal structure correct? Let us just try that.

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Suppose we take, this is a lattice. You take an origin from here this is \mathbf{a} and this is \mathbf{b} . So, this are all the \mathbf{a} planes correct? Is it not? And consider that this is \mathbf{c} which is

perpendicular to the board. So, is it clear you can work it out later? Suppose this is a vector a . These are all the planes which are going to be there these are also this will be a $1\ 0\ 0$ plane this will be $2\ 0\ 0$ plane this will be $1\ \bar{0}\ 0$ correct? Like that these planes will go. Because this is where the planes are which are in the c direction. And these planes will be $1\ 0\ 0$. Now $1\ 0\ 0$ family of planes will come in this look at this are all the family of planes $2\ 0\ 0$ plane cannot come here $2\ 0\ 0$ plane has to come half distance sorry $1\ \bar{0}\ 0$ this will be $1\ 0\ 0$ plane correct?

Now, this is a primitive lattice. What is the plane normal here with respect to this one this is going to be the plane normal to this set of planes correct? To this set of planes like this the plane normal is going to be in this direction. Is it not? Because this is the plane this is the plane the normal to it will vector will come like this that is how the plane normal be with respect to this is $0\ 1\ 0$ correct? Is that clear this is the way we draw a plane normal.

Student: (Refer Time: 45:00).

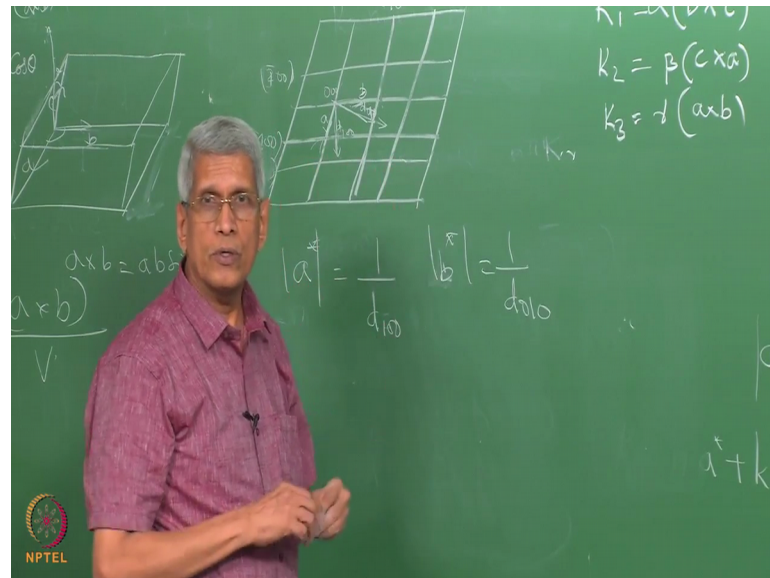
So, see this is if this is a and b are the vectors, this is in $1\ 0\ 0$ direction this is $0\ 1\ 0$ direction this is a parallelogram 2 dimensional this is $1\ 0\ 0$ type of plane family of planes which are there parallel to this one $b\ c$ planes correct? Similarly, the planes which are parallel to this this will be $0\ 1\ 0$ planes the planes which are parallel to this at specific distance along c will turn out to be the $0\ 0\ 1$ plane, because you are always thinking with respect to cubic system. So, you are thinking it has to be perpendicular it is not.

Student: Sir is there the top views are they rotating in top view.

No here what we are doing it here, is I am just showing only a 2 dimensional lattice. If we construct as a 3 dimensional lattice like suppose we assume it is to be a monoclinic system. I can take the next plane will be kept on top of this correct? If you just consider only a 2 dimensional lattice, there are only this is one set of and 3 dimensional lattice if we consider it this is a set of plane, this is a set of plane correct? With respect to this plane what is going to be the normal to it. To this set of planes this is going to be the normal. That is what you have learnt in the real structure is that the vector which represents the direction, and the planes which has the same miller indices, they are plane normal if you consider it. They are not in the same direction correct? That is exactly what we are doing it. So, the between this if you wanted to find out inter planar distance I will have to draw a perpendicular vector no.

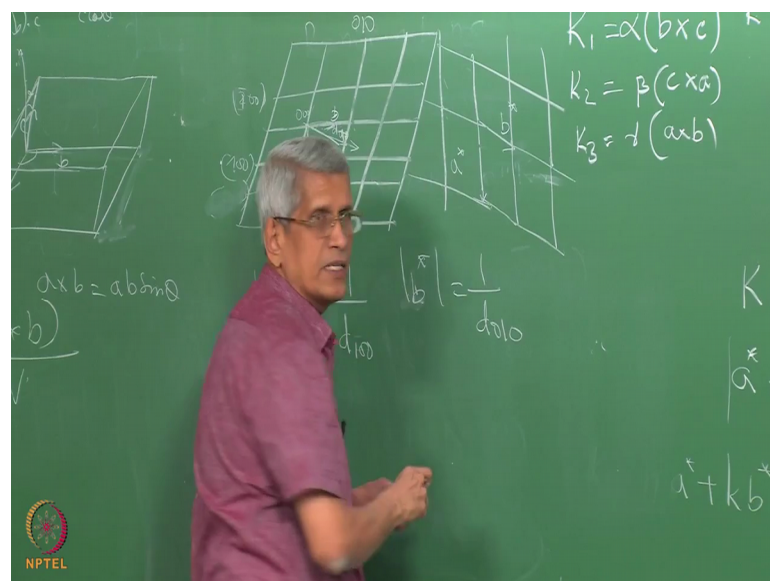
Similarly, if to find out the spacing between these and these directions, essentially these planes are the perpendicular vector. In this vector if I take a distance and suppose this distance is the d_{100} and in this one is d_{100} .

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And if I take the inverse of that distance and mark it on that then, what it will happen a star will be equal to 1 by d_{100} . This are magnitude b star will be equal to 1 by d_{010} d is nothing but the separate the inter particle distance.

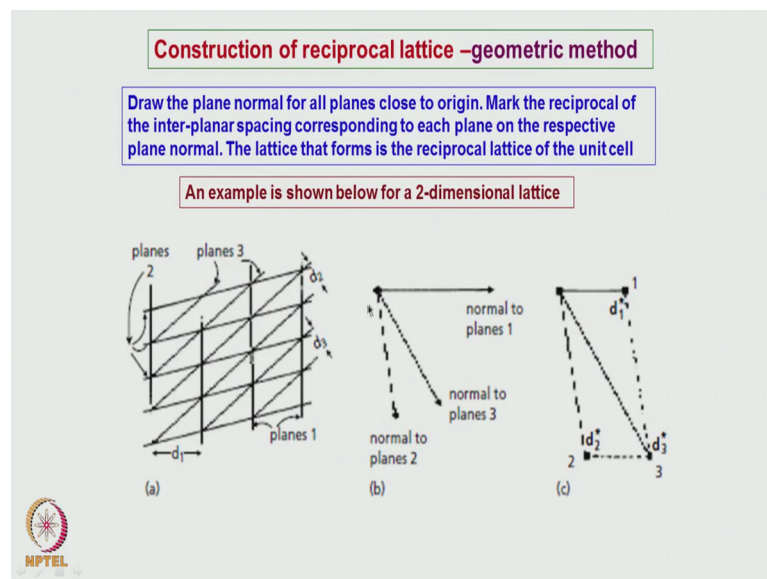
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Now if I try to draw this with respect to these vectors which I have taken. Here, when the plane separation is short the inverse of it will be large correct? So, the vector which we mark as a star here will be proportionately larger and the vector which we will mark as b^* will be proportionately less.

Now, this by vector addition we can generate all other points right. So, that way now we can generate the reciprocal lattice for this 2 dimensional lattice. This is how geometrically we draw it. And in this what we have done it is that which one should always remember is that we have to draw everything with respect to a primitive lattice correct? Suppose in this particular lattice, there is another lattice point here. Then what will happen, the family of planes one plane will come here no, then the separation between the planes is not this it is this separation the distance. So, that is why I said that it automatically takes care of when you take a primitive lattice, it will take care of the factor is taken care of. So, this is how you can draw a simple reciprocal lattice that is what essentially is shown here.

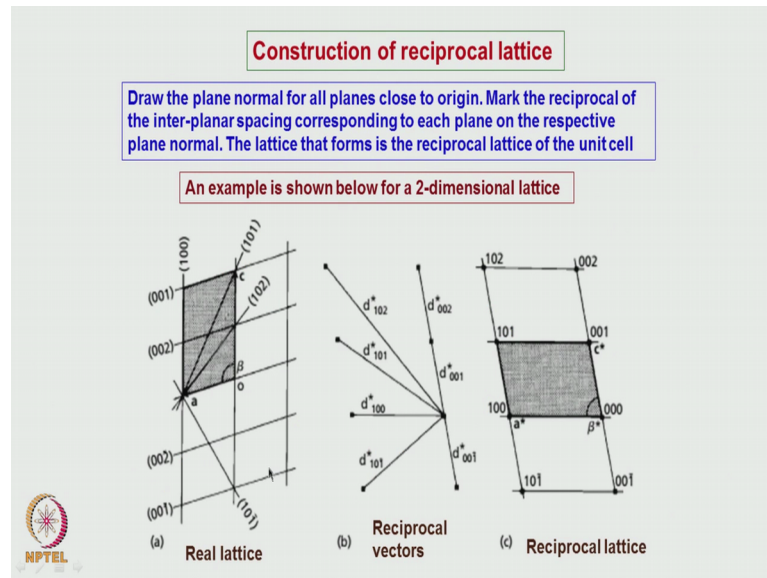
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Draw plane normal, all the planes you can draw the normal and then find out the reciprocal distance and mark it. You have done it this, and the mathematical expression which we have derived it is essentially one and the same we are only implementing the mathematical expression in this from geometrically. So, geometrical way we can construct it, but the problem with happens in geometrical way is that again a 3

dimensional structure, if you wanted to do it becomes little bit more complicated because visualization everything is necessary. Correct? Whereas, when we do it with a mathematical operation from that reconstruction of a lattice is much simpler.

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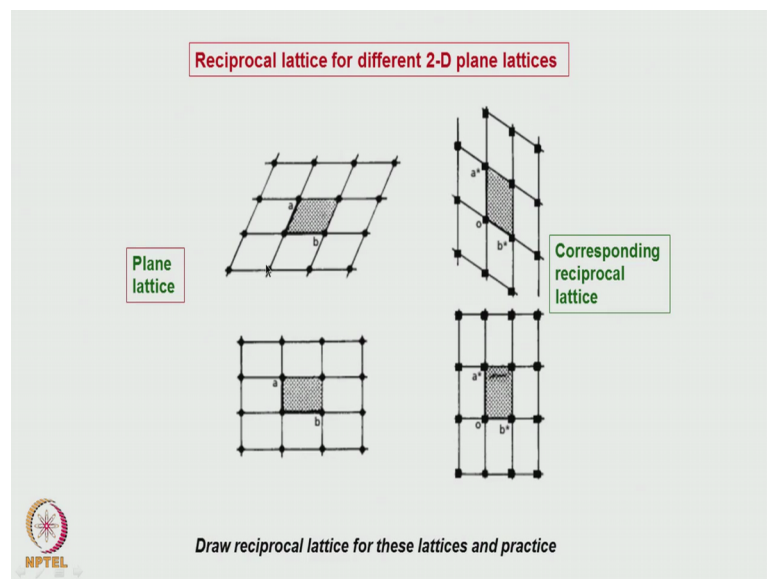
So, that is essentially what is being shown here is the different type of lattices, this is for a parallelogram how the reciprocal lattice vector look like.

But what you should understand if that, these are all when the reciprocal lattice unit cell if you look at it, this unit cell is an (Refer Time: 50:53) at size. Because the distances is in inverse of it, but it is in a space it is an inverse distance correct? So, you can choose some scaling factor to plot it. So, that it is observable to us. What is essentially important is that, taking the like if you when you try to find out the volume of the lattice, in the real lattice it is a dot b cross c right. That volume depends upon what is the unit which we choose to represent a b and c , correct?

Similarly, if you take the reciprocal lattice the reciprocal lattice unit cell it is also we can find out what are the volume is, there the unit is are going to be inverse of the that distance where it is a millimeter or a centimeter or a nanometer inverse of that is that is what we have to take it. If you take the product of these 2 reciprocal lattices this we can work it out as a problem that it will be turning out to be 1. That is volume in real space and volume in reciprocal space of the unit cell perspective unit cells if you consider that products are always going to be 1.

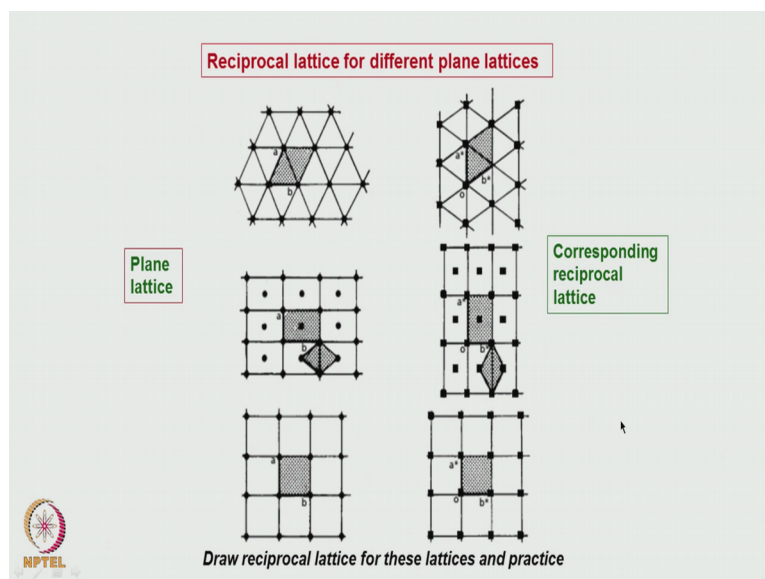
So, this is the one way in which geometrically this also what we will do it is that this time we will have in a real lattice how to construct a lattice. Next week, we will consider how to construct a reciprocal lattice. So, that it will become quite clear how reciprocal lattice can be constructed for any of the Bravais Lattices. Is it clear? That one should become quite familiar with it then it is very easy to understand diffraction pattern and all from various crystal structures. So, this is for the 5 planer lattices are there.

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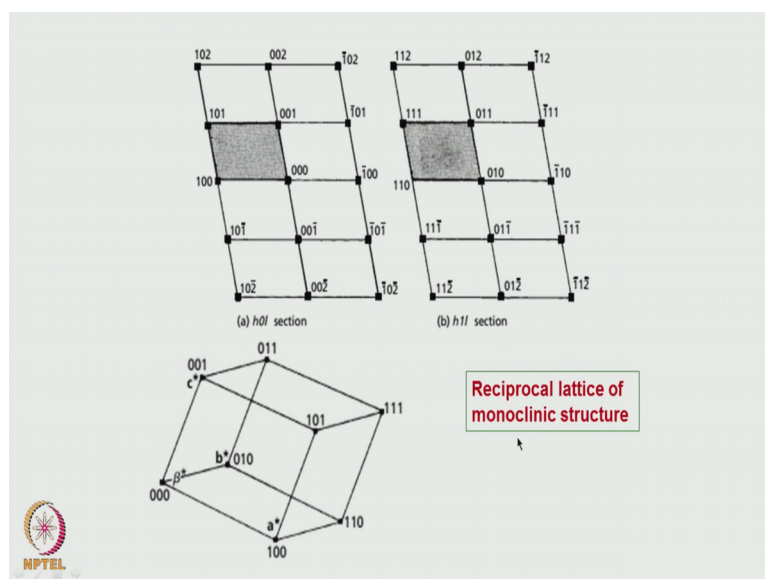


You see this one which we have taken from the book, is these 2 correct? This is the real lattice; this is the reciprocal lattice vector. Are you sure? See this normal should have come like this right. To this planes normal should be here, is it taken that way correct? This one and normal to this should come right. So, similarly if we take a rectangular lattice, how it will be here it is along h in this one it will be in the perpendicular direction it will turn out to be.

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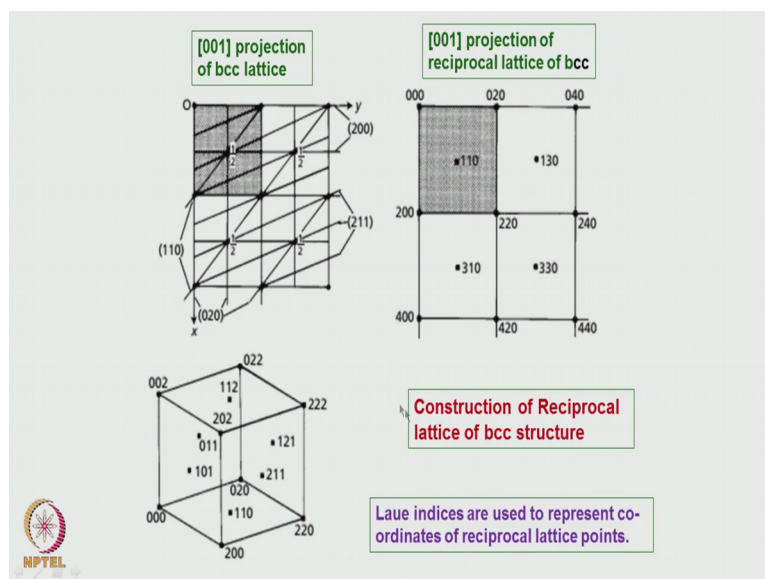
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This is how various reciprocal lattice will appear. So, if we take the lattice the third dimension also, then we can construct a reciprocal lattice unit cell. That is what it has been constructed for a monoclinic system.

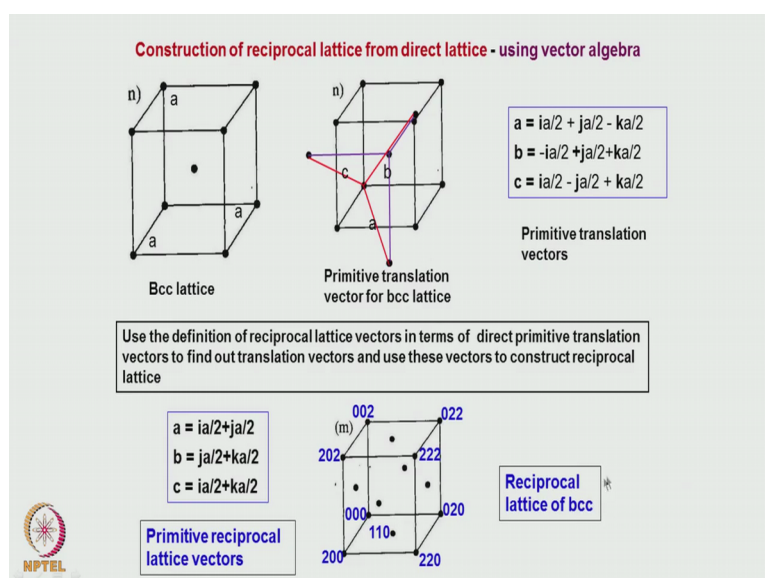
But what is essentially important is that this is one layer, this is another layer which is being put on top of each other, this is what the monoclinic reciprocal lattice has been generated.

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Similarly, one can try to work out for reciprocal lattice for cubic system also cubic and non cubic system, which I think I will give you some assignments to work which you can try it and then we will have class also special class where we will you will try to work out in the class, then it will become quite clear how this reciprocal lattices can be constructed.

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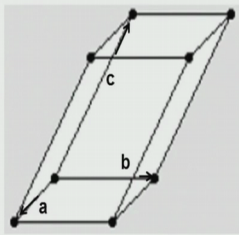


Here just I have shown some with some examples reciprocal lattice, for like for example, we started initially with a cubic system right. This is a body centered lattice BCC, for

which with respect to this point when we try to draw the rhombohedra, that is the primitive lattice this is one vector this is another vector, and this is going to be the third vector. How we take these 3 vectors these are all the coordinates of these vectors. If we try to use a vector algebra, then you will find that that a star b star and c star will turn out to be of this type. Then one can draw the full reciprocal lattice unit cell.

Then if you look at the reciprocal lattice unit what all symmetries which it exhibits it exhibits all the symmetry of the real lattice will be exhibited by the reciprocal lattice also. And here if you see it automatically when you look at some of the reflections, like here 2 0 0 reflection is present right. 1 0 0 reflection is automatically becomes absent because the reciprocal lattice is constructed for a primitive lattice. Similarly, here what I have done it is that how will you find out inter planar distance in a vector notation.

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$$V = a \cdot (b \times c) = (a \times b) \cdot c = b \cdot (c \times a)$$

$$V^* = a^* \cdot (b^* \times c^*)$$

$$c^* = i_c \cdot 1/d_{ab}$$

$$i_c = (a \times b) / |a \times b|$$

$$1/d_{ab} = |a \times b| / V$$

$$d_{ab} = (a \times b) \cdot c / |a \times b|^2$$

$$k = k_1 a^* + k_2 b^* + k_3 c^*$$

$$R = n_1 a + n_2 b + n_3 c$$

$$k \cdot R = k_1 n_1 + k_2 n_2 + k_3 n_3$$

For $e^{-i2\pi k \cdot R} = 1$, $k \cdot R$ should be integer. Since n 's are integer, k 's has to be linear combination of a^* 's with integral coefficients

$$a^* = \frac{b \times c}{V}, \quad b^* = \frac{c \times a}{V}, \quad c^* = \frac{a \times b}{V}$$

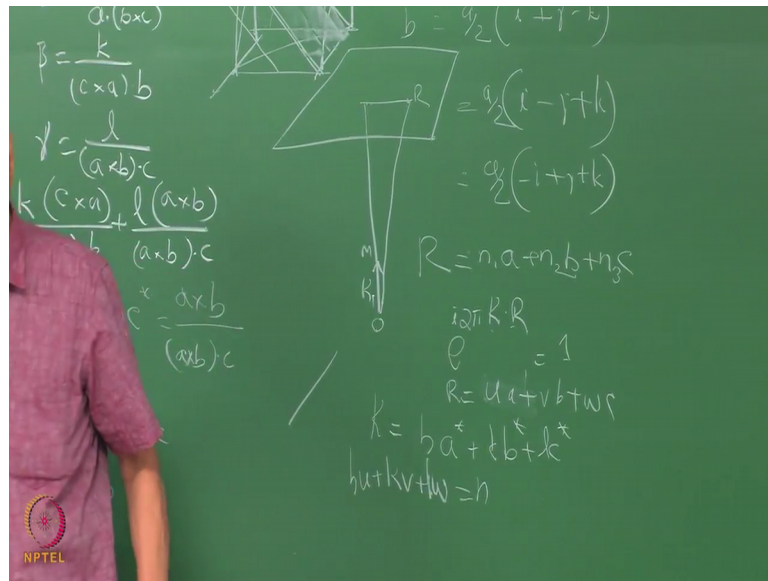
$$a = \frac{b^* \times c^*}{V^*}, \quad b = \frac{c^* \times a^*}{V^*}, \quad c = \frac{a^* \times b^*}{V^*}$$

$$a^* \cdot a = 1; \quad b^* \cdot b = 1; \quad c^* \cdot c = 1$$

$$a^* \cdot b = a^* \cdot c = b^* \cdot c = b^* \cdot a = c^* \cdot a = c^* \cdot b = 0$$

This will be a b into v, divided by a cross b the whole square. That is how it will turn out to be. So, if we summarize what have we done in today's class. What is the way in which real lattice the position in the real lattice can be represented mathematically? That is in a vectorial form.

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If we represent it we generally represent it is r equal n 3 into c correct?

The another form in which it can be represented as a periodic function, if we try to represent it, then it has to be represented in the form of exponential $k \cdot r$ should be equal to 1, where r represents the real lattice vector. Then we try to find out what should be the values of k . What is the relationship between the real lattice vector and the reciprocal lattice vector? So, reciprocal lattice vector essentially represents nothing but planes in real lattice. And then how to construct these lattices just for 2 dimensional lattice has parallelogram we are considered how to draw a reciprocal lattice geometrically.

Both are essentially an equivalent one and in fact, in this equation normally what we write r is equal to r equals u into a plus v into b plus w into c correct? That is how it is represented. And then k we represent it as h in to a^* plus k in to b^* plus l in to c^* correct? If we take that $k \cdot r$ what it will turn out to be it will turn out to be, $h u$ plus $k v$ plus $l w$ right. This turns out to be n no you will be all familiar with this equation is you called as the zone law right. Zone law is also nothing but a relationship between a real lattice and a reciprocal lattice. The reason for this is because whenever we use $h k l$, whether we are aware of it or not when we use $h k l$ to represent the planes it is nothing but using inherently a reciprocal lattice vector is being used because $h k l$ are

nothing but coefficients of reciprocal lattice vector that is why these expression it turns out to be.

These expression normally when it equals 0 is the one which we always say the zone law, but generally there is if we use this law to look at different reciprocal lattice planes if we are able to get that information, that complete crystal structure information will be available from the 3 dimensional lattice that is the Bravais Lattice can be reconstructed from this we will stop here.