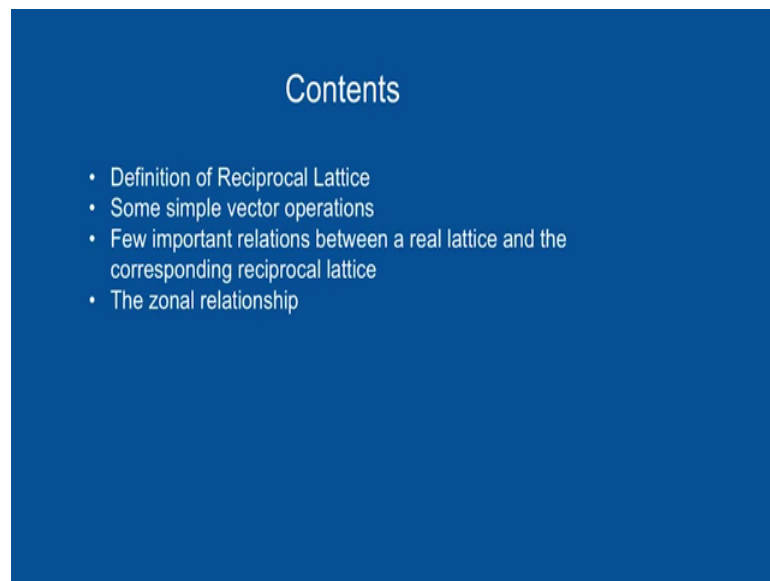


X-Ray Crystallography
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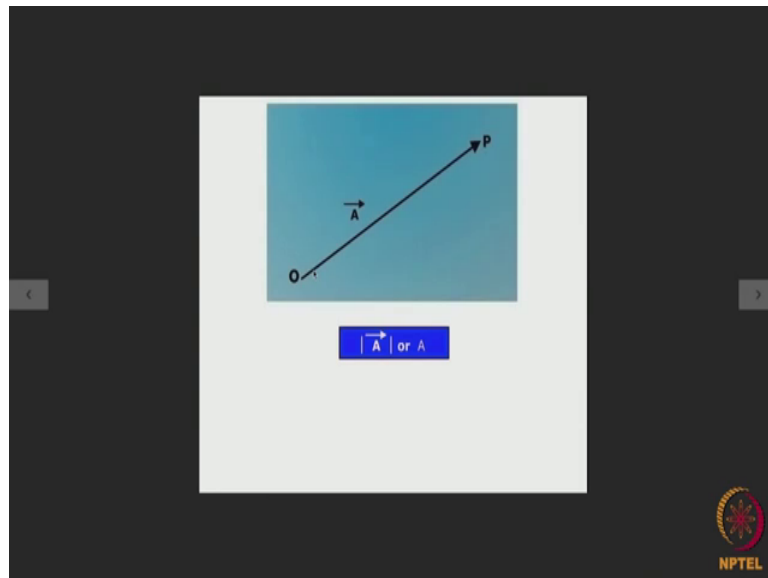
Lecture – 03
Reciprocal Lattice

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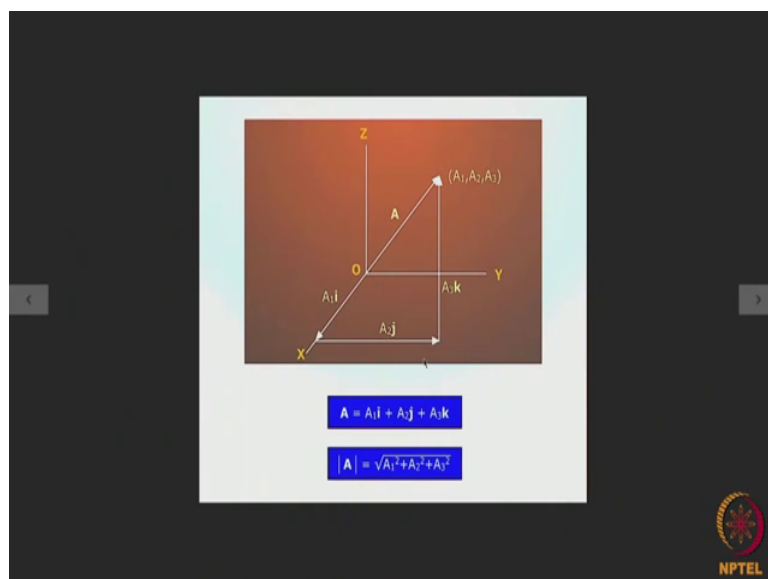
Many important problems related to real crystals can be solved by invoking a mathematical concept known as the reciprocal lattice. Reciprocal lattice exists in an imaginary reciprocal space just as a real lattice exists in real space. There are definite mathematical relationships between a real lattice and its reciprocal lattice. In fact, there are certain reciprocal relationships which do exist between a real lattice and the corresponding reciprocal lattice. I would like to introduce some simple vector operations at this stage as because these will be needed when we get deeper in to the subject.

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Well we all know that a vector has got both a magnitude and a direction. So, in this lecture a letter written in bold will denote a vector otherwise it is a scalar quantity. So, magnitude of the vector A can be written in this manner or it can also be written simply as A .

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Now, any vector in real space can be resolved into 3 components along X , Y , and Z . If i , j , and k these are the unit vectors along the directions X , Y , and Z then a vector A can be resolved into the 3 components namely A_1i , A_2j , and A_3k . So, a vector A can be

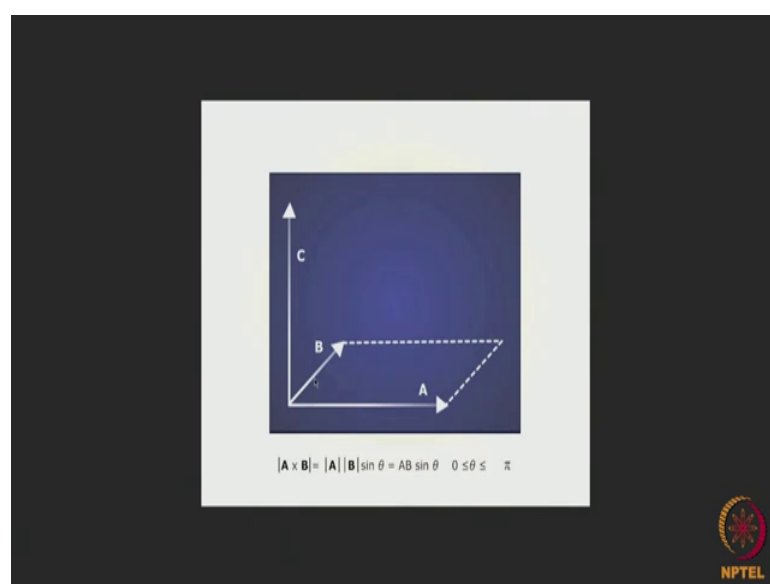
written as $A_1 i + A_2 j + A_3 k$ and the magnitude of the vector A is equal to $\sqrt{A_1^2 + A_2^2 + A_3^2}$.

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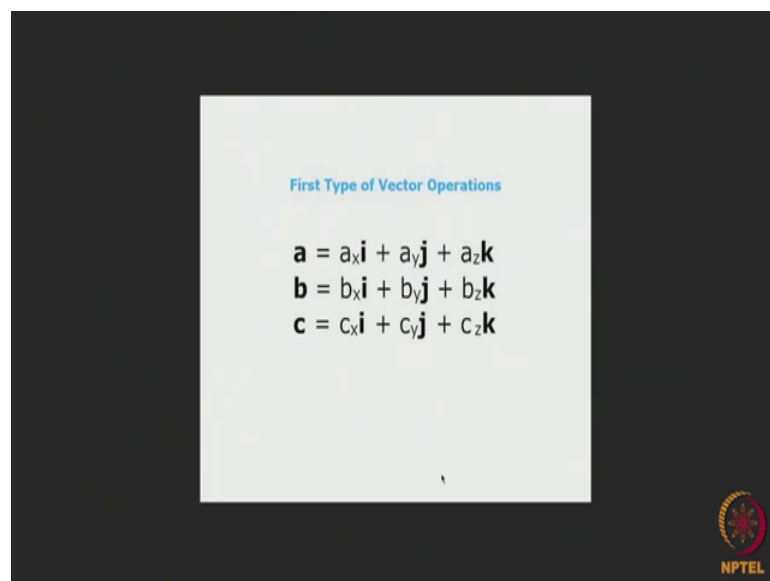
There are 2 types of vector operations which we normally come across suppose A and B are 2 vectors and let the angle between the 2 vectors is θ . So, A dot product the vector B it is a scalar quantity and the magnitude of that is the magnitude of A multiplied by magnitude of B multiplied by cosine θ . So, it will be $AB \cos \theta$.

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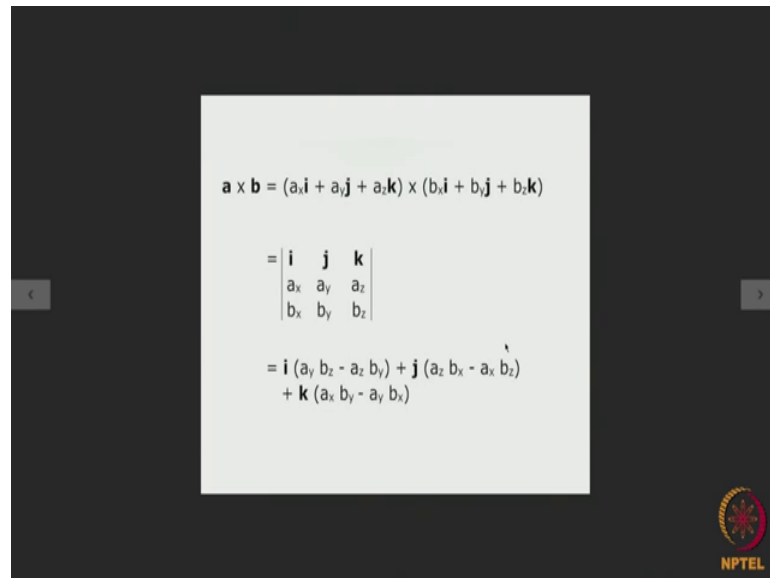
On the other hand there is another product between 2 vectors say for example, this is vector A this is vector B and suppose theta is the angle between the 2 then A cross B is a particular type of product of these 2 vectors and this is equal to a third vector C lying perpendicular to the plane contained by A and B and its direction can be found out from the right handed screw rule. The magnitude of the vector product A cross B is equal to magnitude of A in to magnitude of B multiplied by sin theta that is A B sin theta whereas, the dot product of 2 vectors is a scalar quantity the cross product of 2 vectors is a vector quantity.

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Now, some simple vector operations will be illustrated here. So, we have written down 3 vectors in terms of their components in the X Y and Z direction.

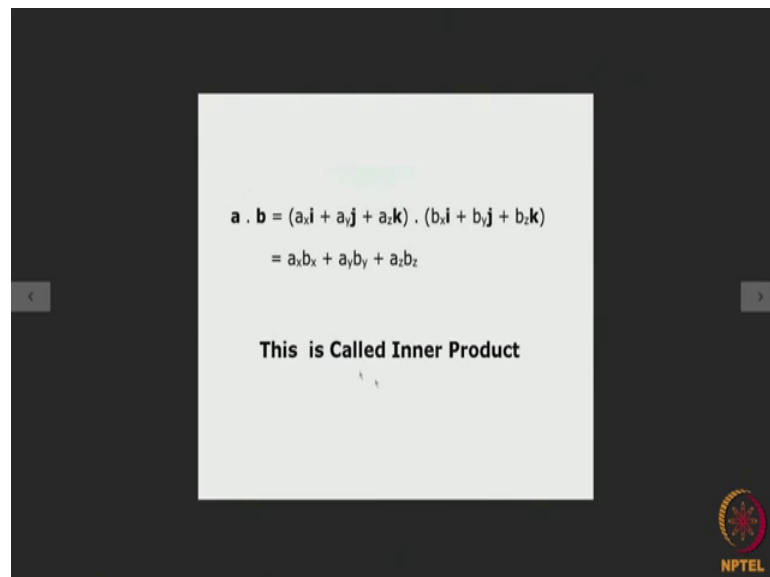
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The slide displays the derivation of the cross product formula. It starts with the vector equation $\mathbf{a} \times \mathbf{b} = (a_x\mathbf{i} + a_y\mathbf{j} + a_z\mathbf{k}) \times (b_x\mathbf{i} + b_y\mathbf{j} + b_z\mathbf{k})$. This is followed by a determinant representation:
$$= \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix}$$
 The final result is:
$$= \mathbf{i}(a_y b_z - a_z b_y) + \mathbf{j}(a_z b_x - a_x b_z) + \mathbf{k}(a_x b_y - a_y b_x)$$

Now, if we make the cross product between the 2 vectors. So, I write these vectors in the confidence. So, it is $a_x \mathbf{i} + a_y \mathbf{j} + a_z \mathbf{k}$ cross product $b_x \mathbf{i} + b_y \mathbf{j} + b_z \mathbf{k}$ and this product can be written simply in a determined form $\mathbf{i} \mathbf{j} \mathbf{k} \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix}$ and then it can also be written in this fashion.

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The slide displays the derivation of the dot product formula. It starts with the vector equation $\mathbf{a} \cdot \mathbf{b} = (a_x\mathbf{i} + a_y\mathbf{j} + a_z\mathbf{k}) \cdot (b_x\mathbf{i} + b_y\mathbf{j} + b_z\mathbf{k})$. This is followed by the simplified result:
$$= a_x b_x + a_y b_y + a_z b_z$$
 Below the equation, it states: **This is Called Inner Product**

And similarly when we make a dot product between 2 vectors \mathbf{a} and \mathbf{b} then we write down the 2 vectors in the form of the components and then the products comes out to be $a_x b_x + a_y b_y + a_z b_z$. Now, this product is also called the inner product.

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$$\begin{aligned}
 (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} &= i(a_x b_z - a_z b_x) + \\
 &\quad j(a_x b_y - a_y b_x) + \\
 &\quad k(a_x b_y - a_y b_x) \cdot (c_x i + c_y j + c_z k) \\
 &= (a_x b_z - a_z b_x) c_x + (a_z b_x - a_x b_z) c_y + (a_x b_y - a_y b_x) c_z \\
 &= \begin{vmatrix} c_x & c_y & c_z \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix} \\
 &= \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} \\
 &= [abc] \\
 (\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} &= (\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a} = (\mathbf{c} \times \mathbf{a}) \cdot \mathbf{b} \\
 [abc] &= [bca] = [cab]
 \end{aligned}$$

Now there is an operation it is 3 vectors say we have we first make a cross product of the vectors a and b. So, the cross product will give us another vector then we make a dot product of that vector with a third vector c. So, it is a cross b dot c. So, how we are going to do that?

Again we you know there will be a third bracket here which is missing, there will be a third bracket here, again we resolve the vectors a b c in to their components and write it as a dot product and this is what it comes up to be a y b z minus a z b y c x plus a z b x minus a x b z c y plus a x b y minus a y b x c z and we can write it down in the determinant form. So, you can interchange the columns and write it in this fashion. Now this product a cross b dot c is also known as what is called the box product and you can write it down in this fashion a b c within the third bracket. It can be shown that a cross b dot c is the same as b cross c dot a is the same as c cross a dot b and you know in this form can be written a b c box product equal to b c a box product in to c a b box product.

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$$\mathbf{a} \times \mathbf{b} = i (a_x b_z - a_z b_x) + j (a_z b_x - a_x b_z) + k (a_x b_y - a_y b_x)$$

$$\mathbf{a} \cdot \mathbf{b} = a_x b_x + a_y b_y + a_z b_z$$

$$(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix}$$

So, now we have learnt how to find out the cross product between 2 vectors, how to find out the dot product between 2 vectors and how to find out products of the type a cross b dot c.

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$$\mathbf{b} \times \mathbf{c} = (b_y c_z - b_z c_y)\mathbf{i} + (b_z c_x - b_x c_z)\mathbf{j} + (b_x c_y - b_y c_x)\mathbf{k}$$

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (a_x \mathbf{i} + a_y \mathbf{j} + a_z \mathbf{k}) \times [(b_y c_z - b_z c_y)\mathbf{i} + (b_z c_x - b_x c_z)\mathbf{j} + (b_x c_y - b_y c_x)\mathbf{k}]$$

$$= a_x(b_y c_z - b_z c_y)\mathbf{k} - a_x(b_z c_x - b_x c_z)\mathbf{j} - a_x(b_x c_y - b_y c_x)\mathbf{i} + a_y(b_z c_x - b_x c_z)\mathbf{k} + a_y(b_x c_y - b_y c_x)\mathbf{i} - a_y(b_y c_z - b_z c_y)\mathbf{j}$$

$$= (a_x b_y c_z - a_x b_z c_y + a_y b_z c_x - a_y b_x c_z + a_z b_x c_y - a_z b_y c_x) \mathbf{i} + (a_x b_z c_x - a_x b_x c_z + a_y b_x c_y - a_y b_y c_z + a_z b_y c_x - a_z b_z c_y) \mathbf{j} + (a_x b_x c_y - a_x b_y c_x + a_y b_y c_z - a_y b_z c_y + a_z b_z c_y - a_z b_x c_x) \mathbf{k}$$

$$= (a_x c_x (b_y + b_z) + a_y c_x (b_z + b_x) + a_z c_x (b_x + b_y) + a_b c_x i + a_b c_x j + a_b c_x k) \mathbf{i} + (a_x c_y (b_z + b_x) + a_y c_y (b_x + b_z) + a_z c_y (b_y + b_x) + a_b c_y i + a_b c_y j + a_b c_y k) \mathbf{j} + (a_x c_z (b_x + b_y) + a_y c_z (b_y + b_x) + a_z c_z (b_x + b_y) + a_b c_z i + a_b c_z j + a_b c_z k) \mathbf{k}$$

$$= (a_x c_x + a_y c_y + a_z c_z) (b_x \mathbf{i} + b_y \mathbf{j} + b_z \mathbf{k}) - (a_x b_x + a_y b_y + a_z b_z) (c_x \mathbf{i} + c_y \mathbf{j} + c_z \mathbf{k})$$

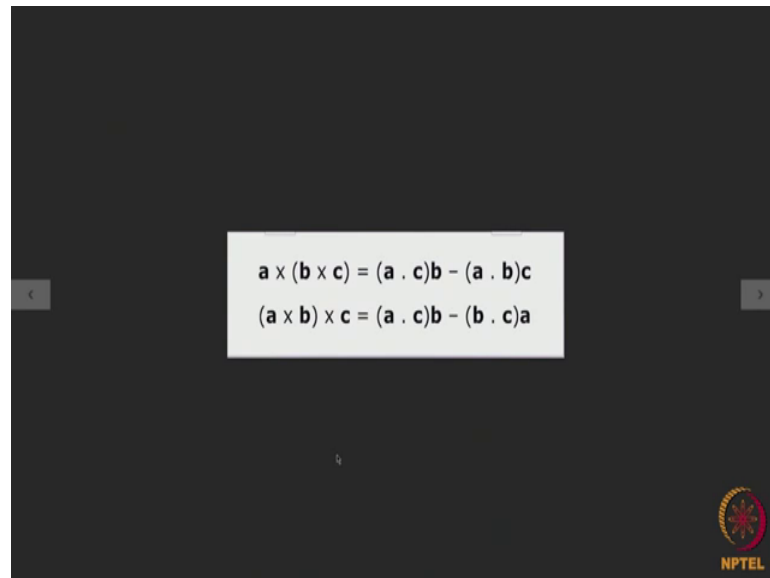
$$= (\mathbf{a} \cdot \mathbf{c}) \mathbf{b} - (\mathbf{a} \cdot \mathbf{b}) \mathbf{c}$$

$$(\mathbf{a} \times \mathbf{b}) \times \mathbf{c} = (\mathbf{a} \cdot \mathbf{c}) \mathbf{b} - (\mathbf{b} \cdot \mathbf{c}) \mathbf{a}$$

Now, let us go to somewhat more complicated problems say for example, we want to find out a cross b cross c. So, b cross c will give us a new vector, so we have to make a cross product of a with that new vector. Again the process is write down all those vectors in terms of their components and do all the operations necessary as shown over here and

once we do that you will find that the product is $a \cdot c b - a \cdot b c$. So, we have now got $a \times b \times c$ is $a \cdot c b - a \cdot b c$. Now if we do it the other way round if we make a cross product between a and b and then the new vector with a makes a cross product with the vector c then this is what it will be - it is $a \cdot c b - b \cdot c a$.

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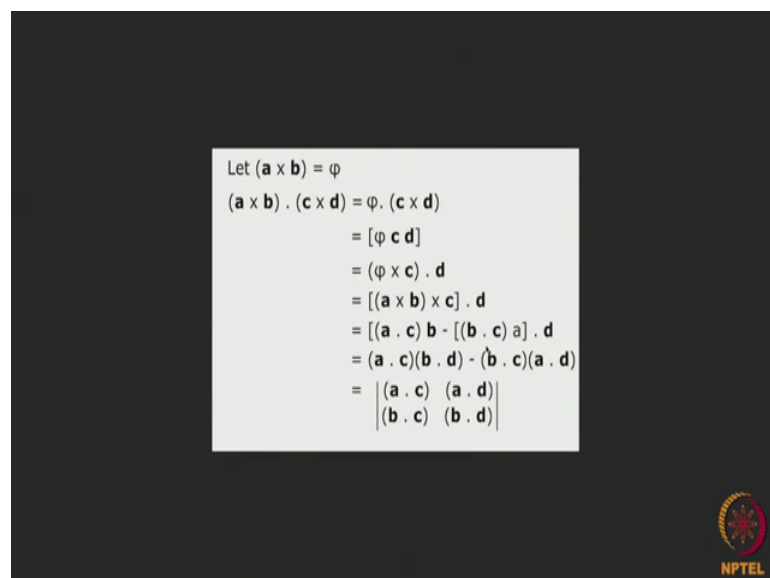


$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{a} \cdot \mathbf{b})\mathbf{c}$$

$$(\mathbf{a} \times \mathbf{b}) \times \mathbf{c} = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{b} \cdot \mathbf{c})\mathbf{a}$$

So, we have found out $a \times b \times c$ is equal to $a \cdot c b - a \cdot b c$ and when it is $a \times b \times c$ then it is $a \cdot c b - b \cdot c a$.

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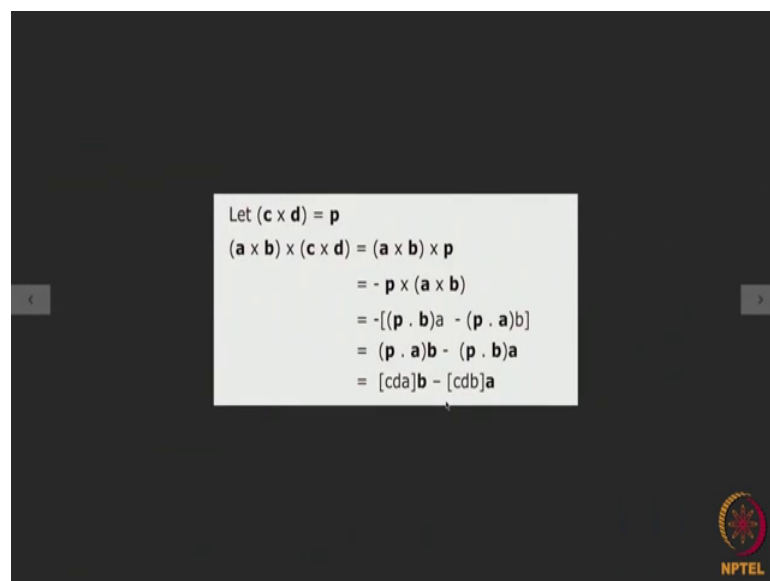


$$\begin{aligned} \text{Let } (\mathbf{a} \times \mathbf{b}) &= \boldsymbol{\phi} \\ (\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) &= \boldsymbol{\phi} \cdot (\mathbf{c} \times \mathbf{d}) \\ &= [\boldsymbol{\phi} \ \mathbf{c} \ \mathbf{d}] \\ &= (\boldsymbol{\phi} \times \mathbf{c}) \cdot \mathbf{d} \\ &= [(\mathbf{a} \times \mathbf{b}) \times \mathbf{c}] \cdot \mathbf{d} \\ &= [(\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{b} \cdot \mathbf{c})\mathbf{a}] \cdot \mathbf{d} \\ &= (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) - (\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \cdot \mathbf{d}) \\ &= \begin{vmatrix} \mathbf{a} \cdot \mathbf{c} & \mathbf{a} \cdot \mathbf{d} \\ \mathbf{b} \cdot \mathbf{c} & \mathbf{b} \cdot \mathbf{d} \end{vmatrix} \end{aligned}$$

Some few more vector operations, somewhat a little bit more complicated ones. Say for example, we want to find out dot product between $\mathbf{a} \times \mathbf{b}$ and $\mathbf{c} \times \mathbf{d}$. Well of course, this will be a vector this will also be a vector. So, how we do it? Say $\mathbf{a} \times \mathbf{b}$ is equal to the vector \mathbf{p} . So, this product will be $\mathbf{p} \cdot \mathbf{c} \times \mathbf{d}$ and naturally it can be written as a box product $\mathbf{p} \cdot \mathbf{c} \times \mathbf{d}$. So, it can be written as $\mathbf{p} \times \mathbf{c} \cdot \mathbf{d}$ and then you know we know what is $\mathbf{p} \times \mathbf{c}$ this is $\mathbf{a} \times \mathbf{b} \times \mathbf{c} \cdot \mathbf{d}$ and we already know the value of this product. So, we write it down and that making a dot product with \mathbf{d} and this will give us $\mathbf{a} \cdot \mathbf{c} \times \mathbf{d} \cdot \mathbf{b} \cdot \mathbf{d} - \mathbf{b} \cdot \mathbf{c} \times \mathbf{d} \cdot \mathbf{a} \cdot \mathbf{d}$. So, in a determinant form it can be written like this.

Let us go in to another kind of vector operation say $\mathbf{a} \times \mathbf{b} \cdot \mathbf{c} \times \mathbf{d}$. Again we put $\mathbf{a} \times \mathbf{b}$ is equal to a vector \mathbf{p} and then proceed in the same manner and we come across the product in the form of a determinant $\mathbf{a} \cdot \mathbf{c} \times \mathbf{d} \cdot \mathbf{b} \cdot \mathbf{d} - \mathbf{b} \cdot \mathbf{c} \times \mathbf{d} \cdot \mathbf{a} \cdot \mathbf{d}$.

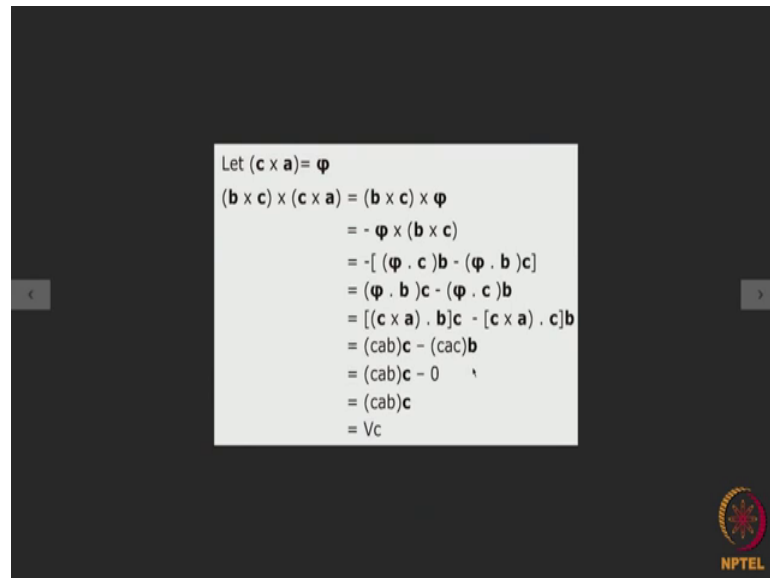
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$$\begin{aligned}
 \text{Let } (\mathbf{c} \times \mathbf{d}) &= \mathbf{p} \\
 (\mathbf{a} \times \mathbf{b}) \times (\mathbf{c} \times \mathbf{d}) &= (\mathbf{a} \times \mathbf{b}) \times \mathbf{p} \\
 &= -\mathbf{p} \times (\mathbf{a} \times \mathbf{b}) \\
 &= -[(\mathbf{p} \cdot \mathbf{b})\mathbf{a} - (\mathbf{p} \cdot \mathbf{a})\mathbf{b}] \\
 &= (\mathbf{p} \cdot \mathbf{a})\mathbf{b} - (\mathbf{p} \cdot \mathbf{b})\mathbf{a} \\
 &= [\mathbf{c} \cdot \mathbf{d} \cdot \mathbf{a}] \mathbf{b} - [\mathbf{c} \cdot \mathbf{d} \cdot \mathbf{b}] \mathbf{a}
 \end{aligned}$$

So, if we want to find out the product $\mathbf{a} \times \mathbf{b} \times \mathbf{c} \times \mathbf{d}$ again you can put the cross product of \mathbf{c} and \mathbf{d} as a new vector \mathbf{p} put it in place here. So, it will be $\mathbf{a} \times \mathbf{b} \times \mathbf{p}$. So, if you want to bring \mathbf{p} on this side it will be $-\mathbf{p} \times \mathbf{a} \times \mathbf{b}$ then it will be you know $\mathbf{p} \cdot \mathbf{b} \cdot \mathbf{a}$ because we know this product minus $\mathbf{p} \cdot \mathbf{a} \cdot \mathbf{b}$. So, it will be finally, the box product of $\mathbf{c} \cdot \mathbf{d} \cdot \mathbf{a} \cdot \mathbf{b} - \mathbf{c} \cdot \mathbf{d} \cdot \mathbf{b} \cdot \mathbf{a}$.


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$$\begin{aligned} \text{Let } (\mathbf{c} \times \mathbf{a}) &= \boldsymbol{\phi} \\ (\mathbf{b} \times \mathbf{c}) \times (\mathbf{c} \times \mathbf{a}) &= (\mathbf{b} \times \mathbf{c}) \times \boldsymbol{\phi} \\ &= -\boldsymbol{\phi} \times (\mathbf{b} \times \mathbf{c}) \\ &= -[(\boldsymbol{\phi} \cdot \mathbf{c})\mathbf{b} - (\boldsymbol{\phi} \cdot \mathbf{b})\mathbf{c}] \\ &= (\boldsymbol{\phi} \cdot \mathbf{b})\mathbf{c} - (\boldsymbol{\phi} \cdot \mathbf{c})\mathbf{b} \\ &= [(\mathbf{c} \times \mathbf{a}) \cdot \mathbf{b}]\mathbf{c} - [(\mathbf{c} \times \mathbf{a}) \cdot \mathbf{c}]\mathbf{b} \\ &= (\mathbf{cab})\mathbf{c} - (\mathbf{cac})\mathbf{b} \\ &= (\mathbf{cab})\mathbf{c} - 0 \\ &= (\mathbf{cab})\mathbf{c} \\ &= V\mathbf{c} \end{aligned}$$

Now, in a similar manner we can find out the cross product between $\mathbf{b} \times \mathbf{c}$ and $\mathbf{c} \times \mathbf{a}$ again we put $\mathbf{c} \times \mathbf{a}$ equal to vector $\boldsymbol{\phi}$ and put it in place here and you know if you change interchange these 2 vectors. So, $\boldsymbol{\phi}$ comes earlier it will be a minus sign here $\boldsymbol{\phi} \times \mathbf{b} \times \mathbf{c}$ and then it will be $\boldsymbol{\phi} \cdot \mathbf{c} \mathbf{b}$ because this product we already know minus $\boldsymbol{\phi} \cdot \mathbf{b} \mathbf{c}$ it will be $\boldsymbol{\phi} \cdot \mathbf{b} \mathbf{c}$ minus $\boldsymbol{\phi} \cdot \mathbf{c} \mathbf{b}$ and then we can find out we can substitute for $\boldsymbol{\phi}$ here. So, it will be $\mathbf{c} \times \mathbf{a} \cdot \mathbf{b} \mathbf{c}$ minus $\mathbf{c} \times \mathbf{a} \cdot \mathbf{c} \mathbf{b}$.

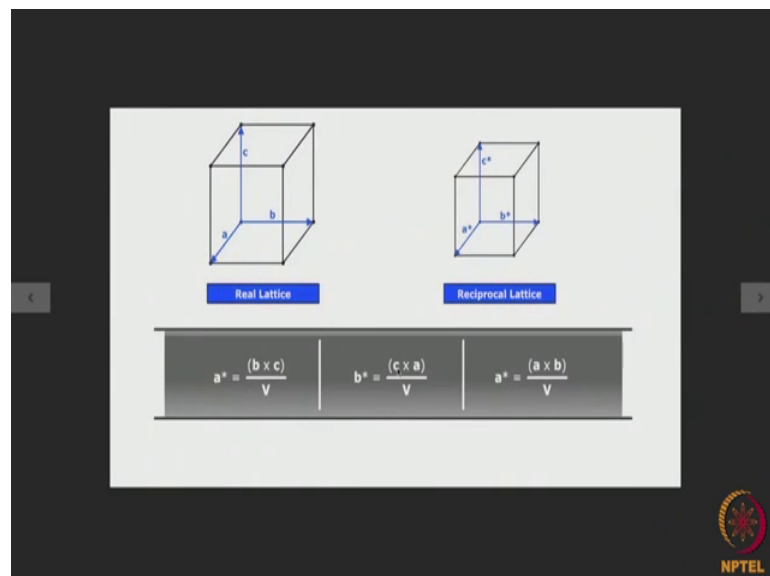
So, this will be equal to the box product $\mathbf{c} \mathbf{a} \mathbf{b} \mathbf{c}$ minus the box products $\mathbf{c} \mathbf{a} \mathbf{c} \mathbf{b}$. Now $\mathbf{c} \mathbf{a} \mathbf{b} \mathbf{c}$ remains as such, but $\mathbf{c} \mathbf{a} \mathbf{c} \mathbf{b}$ you know this box product is simply equal to 0. So, it is $\mathbf{c} \mathbf{a} \mathbf{b} \mathbf{c}$, but you see $\mathbf{c} \mathbf{a} \mathbf{b}$ is what? You know $\mathbf{c} \mathbf{a} \mathbf{b}$ the box product of $\mathbf{c} \mathbf{a}$ and \mathbf{b} . So, if you look at unit cell in the real lattice that real is the volume of the unit cell. So, you can change $\mathbf{c} \mathbf{a} \mathbf{b}$ to V the volume of the unit cell to \mathbf{c} . Now of course, you know it will be a bold \mathbf{c} because this is a vector quantity.

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$$\begin{aligned}(\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) &= \begin{vmatrix} \mathbf{a} \cdot \mathbf{c} & \mathbf{a} \cdot \mathbf{d} \\ \mathbf{b} \cdot \mathbf{c} & \mathbf{b} \cdot \mathbf{d} \end{vmatrix} \\ (\mathbf{a} \times \mathbf{b}) \times (\mathbf{c} \times \mathbf{d}) &= [\mathbf{cda}]\mathbf{b} - [\mathbf{cdb}]\mathbf{a} \\ (\mathbf{b} \times \mathbf{c}) \times (\mathbf{c} \times \mathbf{a}) &= V\mathbf{c}\end{aligned}$$


So, we have found out if we make dot product between the vectors $\mathbf{a} \times \mathbf{b}$ and $\mathbf{c} \times \mathbf{d}$ it can be written in this form the determinant form we also have seen if we do a cross product between the vectors $\mathbf{a} \times \mathbf{b}$ and $\mathbf{c} \times \mathbf{d}$ we can write it in this fashion and if we do cross product of $\mathbf{b} \times \mathbf{c}$ and $\mathbf{c} \times \mathbf{a}$ it will be equal to $V\mathbf{c}$. So, these are some of the important products which you should remember because we may find this from time to time while solving problems using the reciprocal lattice.

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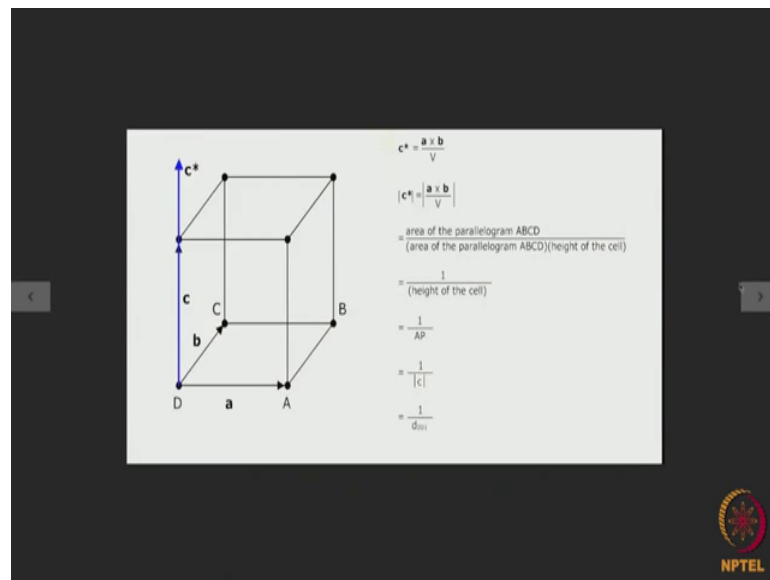
Now, let us come to the relationship between a real lattice and its reciprocal lattice. Say for example, the unit cell in a real lattice is defined by the vectors a , b and c in the X direction, Y direction and Z direction respectively.

Suppose in an imaginary reciprocal space we have got another unit cell which is defined by the vectors a^* , b^* and c^* along the X, Y and Z direction. Now quite arbitrarily it has been chosen that this unit cell if it belongs to a lattice which is reciprocal to this unit cell in the real lattice then a^* will have this kind of relationship with you know b you know the a^* , b^* and c^* , the lattice parameters of the unit cell of the reciprocal lattice will have this kind of relationship with a , b , c you know the vectors which define the unit cell in the real lattice and what is this relationship? a^* is equal to $b \times c$ by V where V is the volume of the unit cell in the real lattice b^* is equal to $c \times a$ by V where V is the volume of the unit cell in the real lattice and it will be c^* I am sorry, c^* is equal to $a \times b$ by V where V is the volume of the unit cell in the real lattice.

So, it seems to me there seems to some madness in to this whole scale why should a^* be equal to $b \times c$ by V b^* should be $c \times a$ by V and c^* should be $a \times b$ by V well there is some method in this madness as we will readily find out. So, you see we should think about the 2 things together a real lattice existing in the real space and a reciprocal lattice existing in an imaginary reciprocal space. So, this is the unit cell of the real lattice this is the unit cell of the reciprocal lattice this is reciprocal to this.

Now we have said quite arbitrarily that the lattice parameters of the unit cell in the real lattice a , b , c and the lattice parameters of the unit cell in the corresponding reciprocal lattice a^* , b^* and c^* are related in this fashion - a^* equal to $b \times c$ by V b^* is equal to $c \times a$ by V c^* it is not a^* here its c^* is equal to $a \times b$ by V . Now we will readily see why you know such relationships have been assumed.

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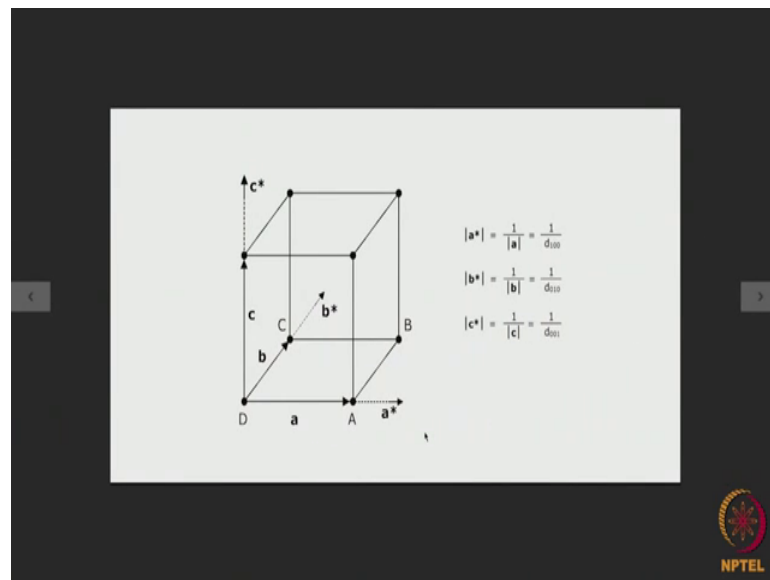


Let us suppose that this is a unit cell in the real lattice, this is a unit cell in the real lattice this is the A vector, B vector and C vector. So, A B and C define the unit cell in the real lattice. Now we have assumed that c star is equal to a cross b by V. So, if this is the unit cell of a cubic lattice and since c star is equal to a cross b by V c star will be pointing in a direction perpendicular to the plane contained by a and b. So, as a result the c star vector will also be along the c vector. So, c star the magnitude is equal to a cross b by V and what is a cross b - is actually the parallelogram area of the parallelogram A B C D. So, this area of the parallelogram is a cross b and what is V? V be the area of the parallelogram A B C D multiplied by the height of the cell. So, the whole volume of the unit cell is this parallelogram multiplied area of this parallelogram multiplied by the height.

So, we can write it down is equal to 1 by AP. So, this is the point P which have not been shown or AP is the same as c. So, we can write it down this is equal to 1 by the magnitude of the vector c. But what is the vector c this length c after all you see c is nothing, but the inter planar distance of the 0 0 1 plane you see this is the 0 0 1 plane and bottom plane is 0 0 bar 1 planes. So, these are parallel planes and the inter planar distance is given by the magnitude of this vector C.

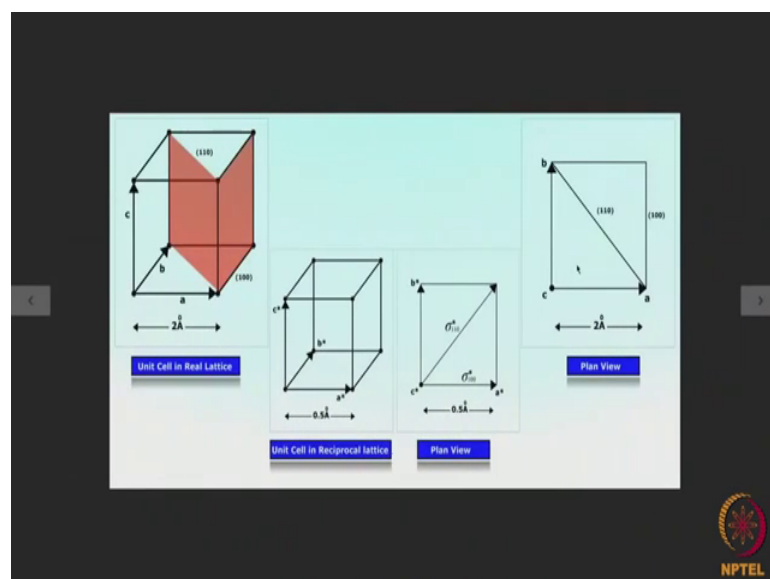
So, we find that the magnitude of the vector c star is actually the reciprocal of the 0 0 of the inter planar distance of the 0 0 1 planes in the real lattice.

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In a similar way we can find out the magnitude of the vector A star is equal to the reciprocal of the inter planar distance of the 1 0 0 planes this is the 1 0 0 plane, this is the backside is a bar 1 0 0 plane. So, this is the inter planar distance. So, magnitude of a star is equal to the reciprocal of the inter planar distance between the 1 0 0 planes then magnitude of b star is equal to the reciprocal of the inter planar distance of the 0 1 0 planes, these are the 0 1 0 planes and c star as we found out earlier is equal the magnitude of c star is equal to the reciprocal of the inter planar distance of the 0 0 1 type planes.

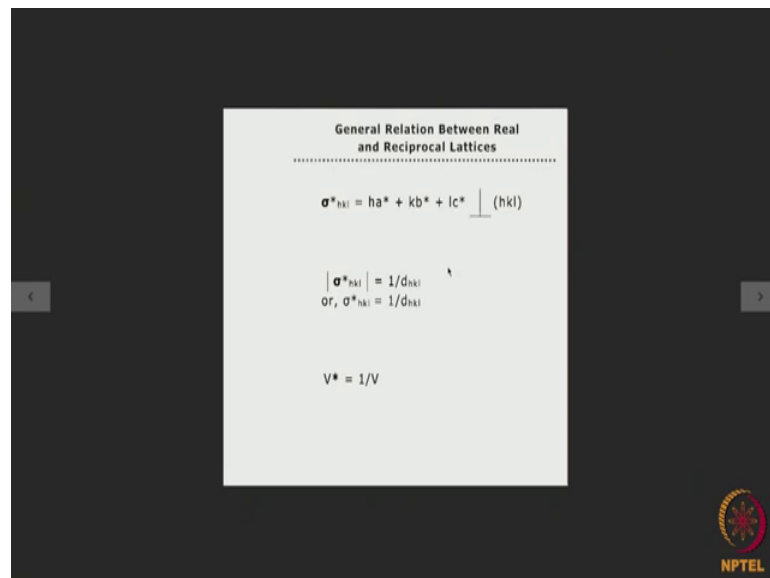
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So, if you have if you thought unit cell in real lattice suppose this is a cubic unit cell in the real lattice and you know say the lattice parameter is 2 angstrom then if you take a plan view of this unit cell say this plane here as we all know is 1 1 0 plane and this right hand side plane here is 1 0 0 plane. So, if we look from the top the plan view then this is what the one the trace of the 1 1 0 plane look like and this will be what the 1 0 0 plane look like. Now correspondingly if we have the unit cell in the reciprocal lattice it is it can be easily found out that the lattice parameter will be equal to 0.5 angstrom we will see why this is so later. And if we take a plan view then if we join this point to that point this is this direction and what is this? This is the direction 1 1 0 in the reciprocal lattice and what about this direction here you know the plan view this is this direction and this is nothing, but the 1 0 0 direction in the reciprocal space.

So, what we find - the 1 1 0 direction in the reciprocal space is perpendicular to the 1 1 0 plane in the real space and 1 0 0 direction in the reciprocal you know space is perpendicular to 1 0 0 plane in the real space. So, some inter relationships can be already found out between a real lattice and its reciprocal lattice.

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Now, there are 3 general relations that can be proved between real and reciprocal lattices. Now the first relationship is if we draw a vector sigma star hkl from the origin of the reciprocal lattice to a point hkl in it then that vector can be simply written down in to its components ha star plus kb star plus lc star please remember a star b star and c star

should be bold and these are vectors. So, the vector σ^*_{hkl} it is 3 components are $h\mathbf{a}^*$ plus $k\mathbf{b}^*$ plus $l\mathbf{c}^*$. So, this vector in the reciprocal lattice will be perpendicular to the hkl plane in the real lattice in the previous diagram we have already seen such a thing. So, the first relationship that exists between a real and the reciprocal lattice are any vector σ^*_{hkl} in the reciprocal lattice starting from the origin of the reciprocal lattice to a point hkl in it will be perpendicular to the hkl plane in the real lattice.

Not only that the second relationship is the magnitude of the vector σ^*_{hkl} will be equal to the reciprocal of the inter planar distance of the hkl planes this is the second relationship we can write it simply as σ^*_{hkl} is equal to $1/d_{hkl}$. And the third relationship is that V^* volume of the unit cell in the reciprocal lattice is equal to reciprocal of the volume of the unit cell in the real lattice. So, these 3 relationships we are going to prove now.

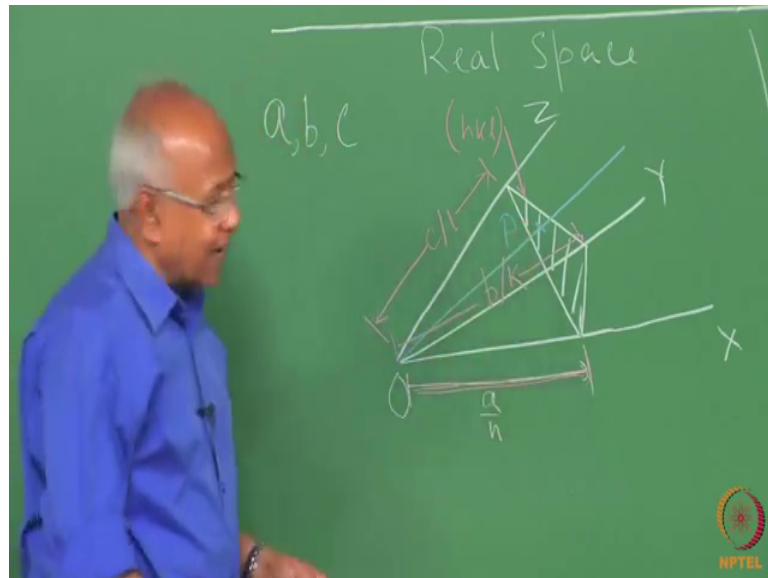
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$OA = \frac{a}{h}, OB = \frac{b}{k}, OC = \frac{c}{l},$
 $AB = OB - OA = \left(\frac{b}{k} - \frac{a}{h}\right)$
 $AC = OC - OA = \left(\frac{c}{l} - \frac{a}{h}\right)$
 $\sigma^*_{hkl} \cdot AB = (ha^* + kb^* + lc^*) \cdot \left(\frac{b}{k} - \frac{a}{h}\right)$
 $= k\left(\frac{1}{k}\right) - h\left(\frac{1}{h}\right)$
 $= 1 - 1$
 $= 0$
 σ^*_{hkl} is perpendicular to **AB**
 $\sigma^*_{hkl} \cdot AC = (ha^* + kb^* + lc^*) \cdot \left(\frac{c}{l} - \frac{a}{h}\right)$
 $= l\left(\frac{1}{l}\right) - h\left(\frac{1}{h}\right)$
 $= 1 - 1$
 $= 0$
 σ^*_{hkl} is perpendicular to **AC**
 σ^*_{hkl} is perpendicular to plane ABC or plane (hkl)

Say for example, we take any kind of unit cell in the real lattice, say we have a real lattice you know and we consider this is the X axis this is the Y axis and this is the Z axis and same the lattice parameters of the unit cell are simply A B and C. Now if we plot a plane A B C in this real lattice and if it is an hkl plane then what will happen? This intercept will be equal to a by h , this intercept will be equal to b by k ; this intercept will be equal to c by l .

We know that if you have a plane hkl and if it cuts the X Y and Z axis along at the points A B and C in that case the intercepts will be a by h along X, b by k along Y and c by l along Z. Now suppose through the point O we draw a straight line parallel to the vector σ^*_{hkl} in the reciprocal space. So, what essentially we are doing?

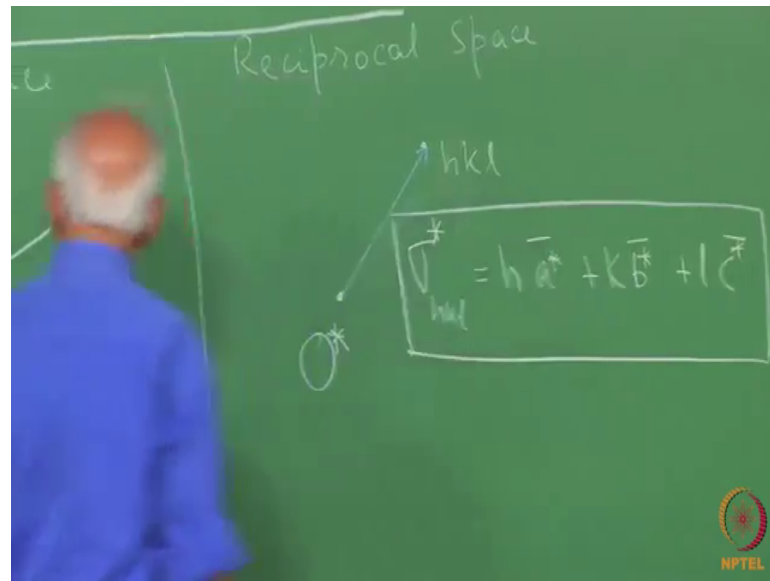
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We have got a real space and at the same time we have got a reciprocal space. So, we have got a situation like this these are the X Y and Z axis and suppose we have got a situation that we have got an hkl plane over there. So, if it is an hkl plane and if a , b and c are the lattice parameters then; obviously, from the origin this distance will be equal to a by h . So, this distance will be equal to a by h .

Similarly, this distance over here from here will be equal to b by k and this distance over here will be equal to c by l then only this will be an hkl plane. So, if we consider this as an hkl plane in the real lattice and if a , b , c are the lattice parameters along X Y and Z then the intercept of the hkl plane on the X axis will be a by h , intercept on the Y axis will be b by k , intercept on the Z axis will be c by l .

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Now, side by side we can construct a reciprocal space and imaginary space and suppose we have got the origin of the reciprocal space denoted by the point O^* just as the origin in case of the real space is O . Now say this is the point hkl this is the point hkl in the reciprocal space this is the point hkl reciprocal space. So, if from the origin of the reciprocal space we draw a line to hkl , so if we draw a line to hkl then what is this vectors going to be? We call this vector as σ^*_{hkl} ; we name this vector σ^*_{hkl} . So, naturally any vector it can resolve 3 components.

So, in the reciprocal lattice you can resolve the vector along a^* , along b^* and along c^* . So, we can write down this as a vector $h a^*$ you know $h a^*$ plus $k b^*$ plus $l c^*$. So, now, what we are going to proof? We are going to proof that this vector in the reciprocal lattice is going to be perpendicular to the hkl plane in the real lattice. So, what we do over here? Through the origin of the reciprocal of the real lattice we draw a line parallel to this σ^*_{hkl} line. So, what we do essentially is from the origin of the real lattice we draw the line parallel to σ^*_{hkl} in the reciprocal lattice.

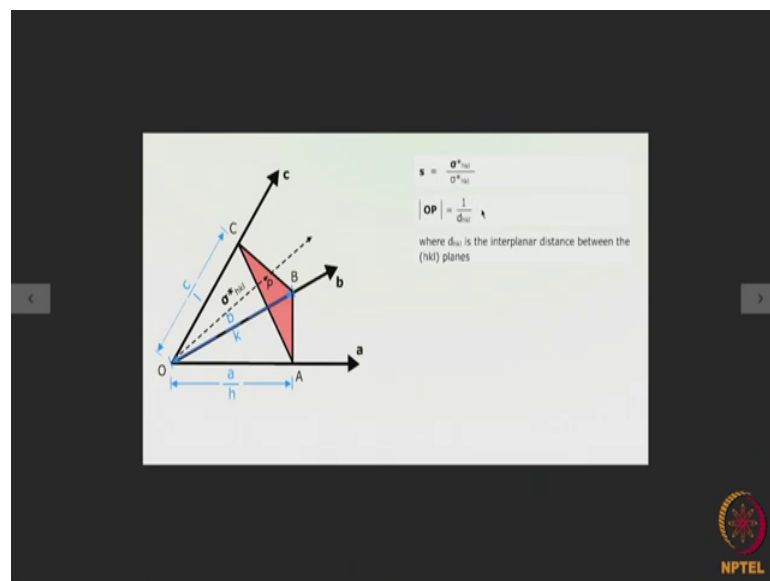
So, suppose we do that I will suppose it cuts the hkl plane at the point p , suppose it cuts the hkl plane at the point p . So, we have a situation that we have a vector σ^*_{hkl} in the reciprocal space which is equal to $h a^*$ plus $k b^*$ plus $l c^*$ and in the real lattice we have got an hkl plane we draw a line from the origin of the real lattice parallel

to you know a vector parallel to the sigma star hkl vector in the reciprocal lattice and suppose this cuts the hkl plane at the point p.

Now since OA is equal to a by h. So, we can write down since OA is a by h, OB is b by k, OC is c by l. So, in vectorial notation you can write OA is equal to a by h - a being a vector, OB vectors is equal to b by k - b being a vector, OC is equal to c by l - c being a vector. So, AB vector is equal to OB minus OA. So, it will be equal to b by k minus a by h and AC will be equal to OC minus OA equal to c by l minus a by h.

Now if we take a dot product between the sigma star hkl vector and the AB vector we can write down in to the components of sigma star hkl, the component you know in the component form we can write down sigma star hkl is equal to ha star plus kb star plus lc star and is a dot product b by k minus a by h. Now if we do the dot product it becomes equal to 0 and what does that indicate? If the dot product is 0 that shows that sigma star hkl vector is perpendicular to the vector AB. In a similar manner if we do the dot product between sigma star hkl vector and the vector AC we can again write down in its component form ha star plus kb star plus lc star dot c by l minus a by h it is again becoming 0, that means, sigma star hkl vector is perpendicular to AC also. So, we see that sigma star hkl vector is perpendicular to the vector AB as well as to the vector AC, on other words sigma star hkl vector is perpendicular to the plane ABC or the plane hkl. So, the first relationship that we mentioned earlier is proved.

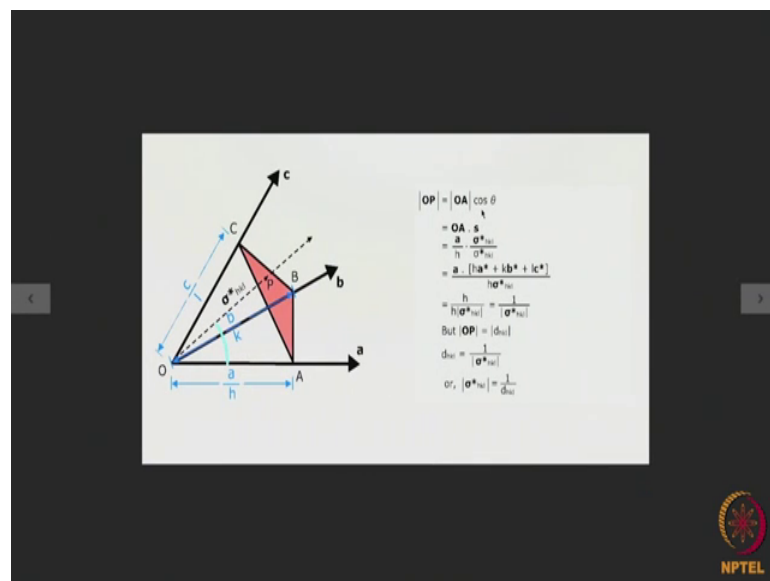
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Now, let us go to the second relationship you see this length this is the vector parallel to the sigma star hkl vector. So, if we find out this length OP, how much is OP? It is erroneously written here as 1 by d hkl actually it will be simply d hkl, you see OP is nothing, but the inter planar distance of hkl type of planes. So, this is an hkl type of plane, here will be parallel hkl type of plane, so the distance between the 2 this OP is actually the inter planar distance of hkl type of planes. So, the magnitude of OP is simply d hkl not 1 by d hkl this is wrong you know, there should be a correction. So, magnitude OP is simply equal to d hkl.

Now let us consider a unit vector s along OP. So, if we say there is a unit vector along OP what it means? Unit vector means after all this is the sigma star hkl vector, this vector is parallel to and equal to the sigma star hkl vector. So, unit vector along this direction is nothing, but the sigma star hkl vector divided by the magnitude of the vector. So, we will be using these 2 relationships. Please remember that the magnitude of OP is simply d hkl and not what is written here.

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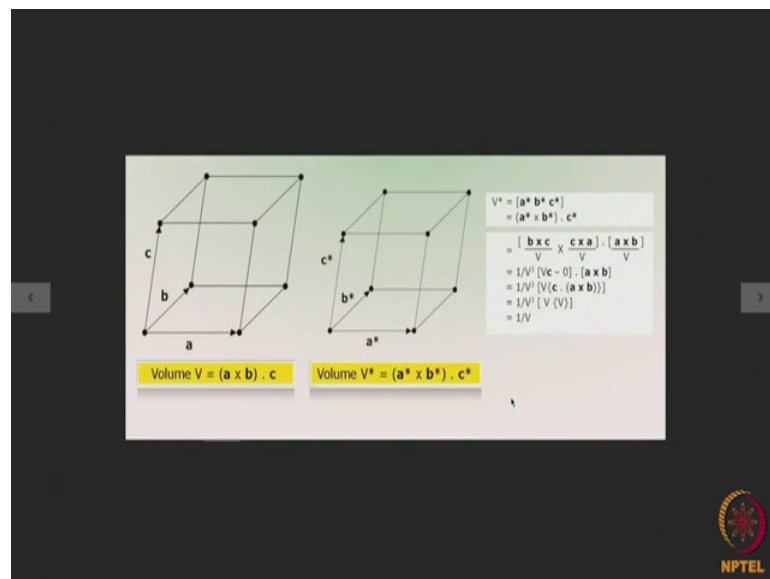


Now, let this angle between OP vector and OA vector be equal to theta. Now what is OP vector? OP vector you can write it as OA vector in to cosine theta OP vector is nothing, but OA vector to cosine theta you know from this right angle triangle. So, it is equal to we can also write it as OA vector dot s the unit vector along OP is the same thing. So, how much is this OA is the vector A by h dot product what is s? The unit vector along

sigma star hkl. So, it is sigma star hkl divided by magnitude of sigma star hkl and then is equal to a dot you know now we write down the sigma star hkl vector in to its components, so it is ha star plus kb star plus lc star and you know in the denominator we have h and the magnitude of sigma star hkl only. So, you know this sigma should be in lower case you see it is not a vector as we can see over here.

So, this is equal to h divided by h the magnitude of sigma star hkl; that means, this will be one by magnitude of sigma star hkl, but already have seen that OP is d hkl. So, OP is already we have found out that is d hkl and at the same time what we find OP is 1 upon the magnitude of sigma star hkl. So, d hkl is equal to 1 by magnitude of sigma star hkl. So, we can write the magnitude of the vector sigma star hkl is equal to 1 upon d hkl. So, this is what we wanted to prove as a second relationship between a real lattice and the reciprocal lattice.

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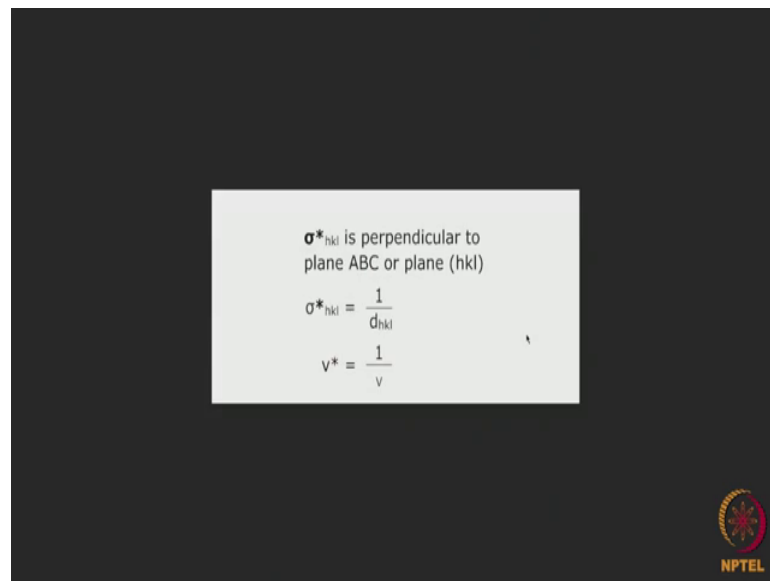
Now, comes the third relationship between a real lattice, and a unit cell in the real lattice and unit cell in the corresponding reciprocal lattice. Say this is the unit cell in the real lattice its volume is V and V can be written as the vectors a cross b and dot product between this and the vector c.

Similarly if this is the unit cell in the reciprocal lattice, this is the corresponding unit cell in the reciprocal lattice then it is defined by the vectors a star b star and c star. So, the volume of the unit cell b star can be written as the cross product a star plus b star and dot

product of this with the vector c^* . So, easily we can write the volume b^* is the box product of the 3 vectors $a^* b^* c^*$. So, this is equal to $a^* \times b^* \cdot c^*$ now we know that a^* is equal to $b \times c$ by V and b^* is $c \times a$ by V and c^* is $a \times b$ by V . So, we have got 1 upon V^3 and this product we know is $V^3 \cdot c \cdot a \times b$ and this is 1 by $V^3 \cdot V^3 \cdot c \cdot a \times b$ and we know that $c \cdot a \times b$ is again V . So, it will be 1 by V^3 multiplied by V in to V ; that means, it becomes 1 by V .

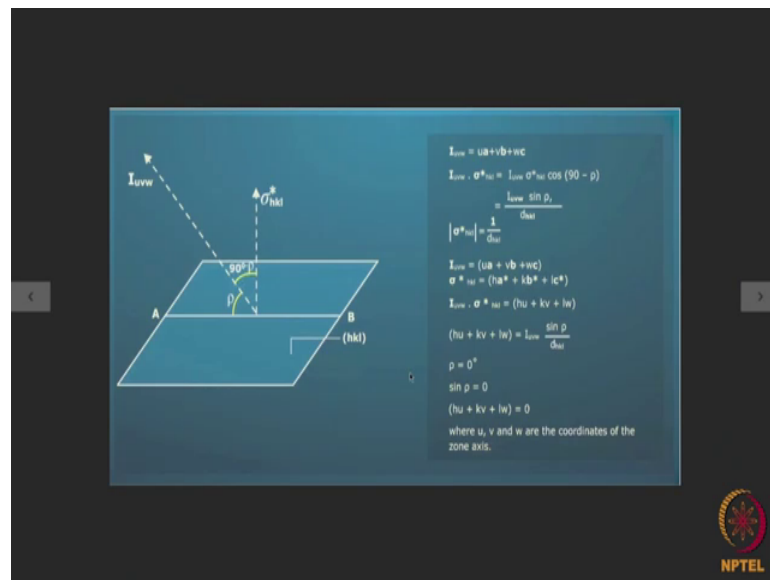
So, the volume of the unit cell in the reciprocal lattice is the reciprocal of the volume of the unit cell in the real lattice. So, these are 3 very important relationships which exist between a reciprocal lattice and a corresponding real lattice or between a real lattice and the corresponding reciprocal lattice.

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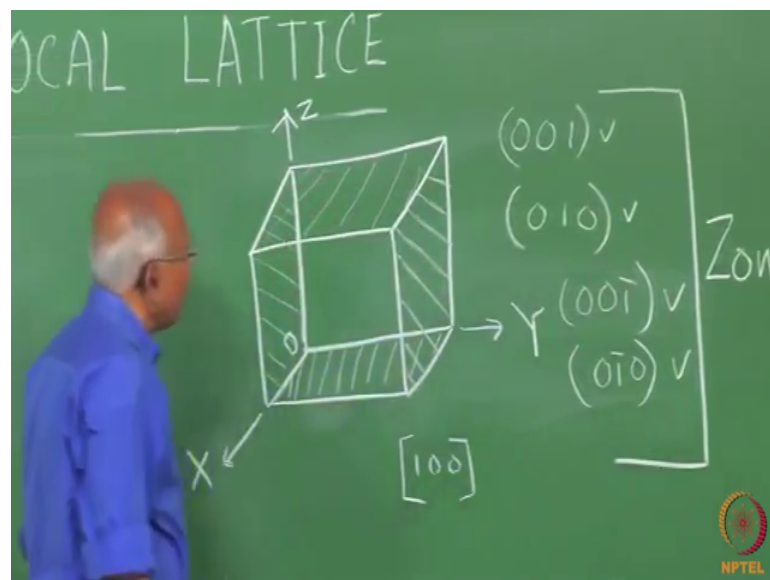
So, we have proved that a vector σ^*_{hkl} in the reciprocal lattice is perpendicular to the plane hkl in the real lattice, the magnitude of the vector σ^*_{hkl} is the reciprocal of the inter planar distance of the hkl planes and the volume of the unit cell in the reciprocal lattice is a reciprocal of the volume of the unit cell in the real lattice.

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We are now going to prove another very important relationship using the reciprocal lattice concept and this is the concept of a zone of planes and the zone axis.

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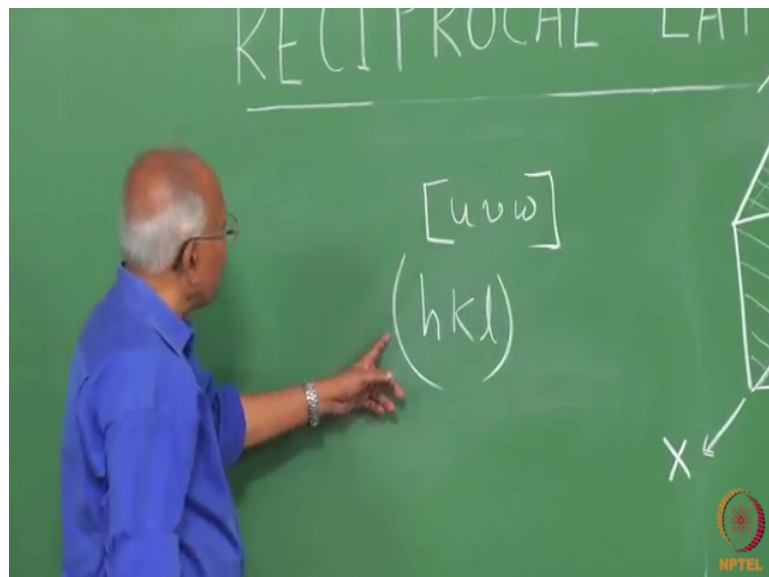


Now, suppose this is a cubic unit cell in the real lattice, now if we look at the top plane over here we know that the top plane is the 0 0 1 plane, if we take the right hand side plane here this is the 0 1 0 plane, if we talk about the bottom plane here it will be the 0 0 bar 1 plane and if we look at the left hand side plane here it will be the 0 bar 1 0 plane. So, the top plane, the right hand side plane, the bottom plane and the left hand side plane,

each one of them is parallel to an axis perpendicular to the plane of the board; that means, what is this direction? This direction in the cubic unit cell is nothing, but the 1 0 0 direction, this is the 1 0 0 direction, 1 0 0 direction is perpendicular to the 1 0 0 plane.

So, what we find that these four planes each one of them is such that it is parallel to the direction 1 0 0 the same direction. In such a case we say that these four planes they belong to one zone, we say that these four plane belong to one zone and this direction with which they are parallel to is known as the zone axis. So, this is a very important relationship in crystallography.

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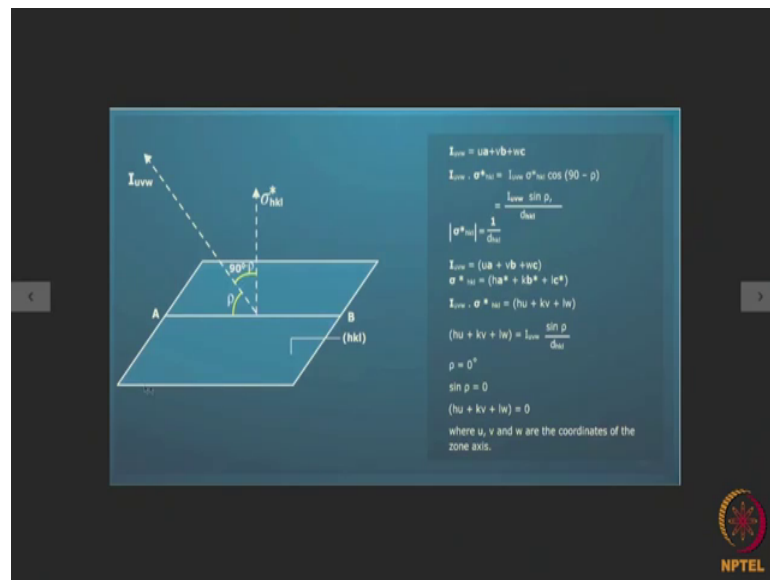


Similarly if we look at the front plane, the right hand side plane, the back plane and the left side plane, all four planes are parallel to this axis which is the 0 0 1 direction. So, this plane, this plane, the bottom plane and the front plane right, hand side plane, back plane and left hand side plane they are all parallel to the 0 0 1 direction. So, those four planes also form a zone with this direction of the zone axis.

Now, we are going to proof a relationship and find out what relationship exists between zone and zone axis and if a given zone axis is given say, if a zone axis is designated as uvw using the relationship which we are going to proof we can easily find out whether a plane hkl will belong to a zone for which this is the zone axis.

Now, let us see how to proceed with this.

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Say for example, we have a plane hkl plane in the real lattice, this is the line on the plane say this is a direction perpendicular to the plane and I have written σ^*_{hkl} this is very clear because we have already seen that if we have an hkl plane in the real lattice then the vector σ^*_{hkl} in the reciprocal lattice is going to be perpendicular to this plane. Let us inscribe a line you know called I_{uvw} . So, this point is the uvw point. So, this vector I_{uvw} connects this point origin to the point uvw in the real lattice. Now this line, this line and this line are say coplanar say. Suppose this angle between I_{uvw} and a is ρ in that case this angle between I_{uvw} and σ^*_{hkl} will be 90° minus ρ .

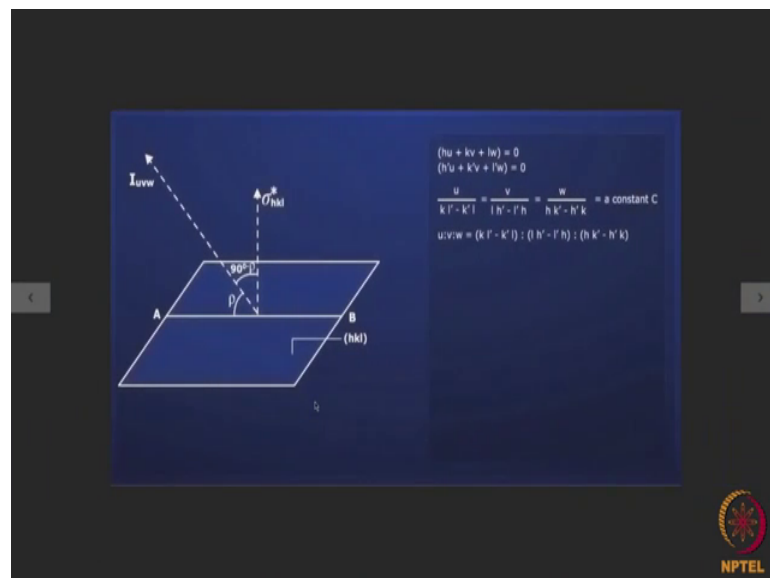
So, now, we can write down I_{uvw} vector is in the real space it is equal to $ua + vb + wc$. So, if we make a dot product of I_{uvw} and σ^*_{hkl} then it will be I_{uvw} magnitude of that σ^*_{hkl} magnitude of that in to cosine of 90° minus ρ . So, it will be magnitude of I_{uvw} in to $\sin \rho$ and since this is equal σ^*_{hkl} is equal to $1/d_{hkl}$ we can write it in this fashion it will be $I_{uvw} \sin \rho$ by d_{hkl} . So, again you know that σ^*_{hkl} the magnitude is nothing, but its magnitude equal to $1/d_{hkl}$. So, I have written instead of σ^*_{hkl} I have written $1/d_{hkl}$.

Now if you write down I_{uvw} in to its component vectors it will be $ua + vb + wc$ and if we write down the σ^*_{hkl} vector in reciprocal lattice it is in to its components it will be $ha^* + kb^* + lc^*$. So, if we make a dot product

between these 2 it can be easily seen that the dot product will be $hu + kv + lw$. So, we see that the dot product between these 2 vectors is equal to $hu + kv + lw$ and again the dot product between these 2 vectors is equal to $I_{uvw} \sin \rho$ by d_{hkl} . So, we equate these 2 if ρ is equal to 0 $\sin \rho$ will be automatically 0 and $hu + kv + lw$ will be 0, you see $\rho = 0$ means that this plane hkl plane will be parallel to the direction I_{uvw} . So, the hkl plane you know and uvw direction will be parallel and the condition is $hu + kv + lw$ is equal to 0.

So, if hkl plane belongs to a zone as where uvw is the zone axis then the relationship must be $hu + kv + lw$ is equal to 0 otherwise this plane will not belong to the zone uvw .

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So, using this relationship we can find out quite a few things. Say for example, we have got 2 planes hkl and $h'k'l'$ belonging to the same zone for which the zone axis is uvw . So, using that relationship the zonal relationship we can write down $hu + kv + lw$ is equal to 0, $h'u + k'v + l'w$ is equal to 0 and so by cross multiplication we can find out u divided by this is equal to v divided by this is equal to w divided by this.

So, u is to v is to w is equal to this quantity, is to this quantity, is to this quantity and these are known quantities because I know I have been given those 2 planes so I can easily find out what uvw are going to be. So, you see that using the zonal relationship we

can find out whether a particular plane will belong to a particular zone having a particular zone axis, not only that if we know more than one planes which belong to a zone then using the zonal relationship we can also find out what should be the zone axis.