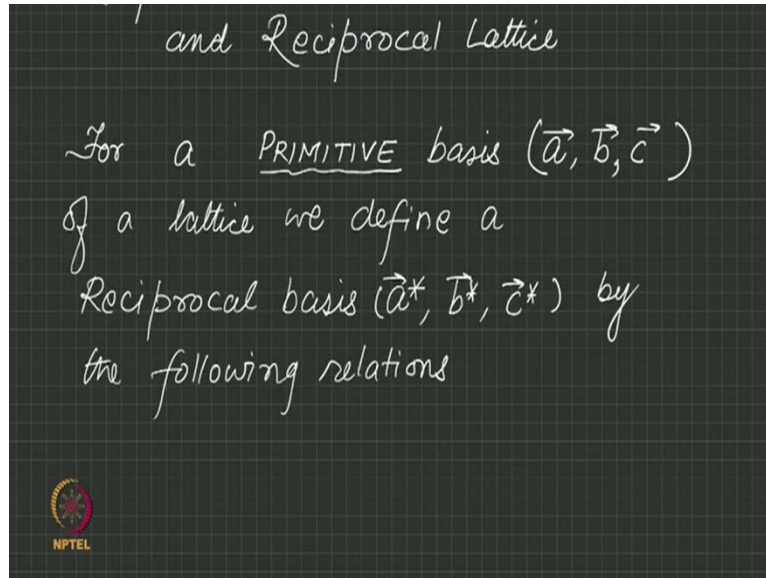


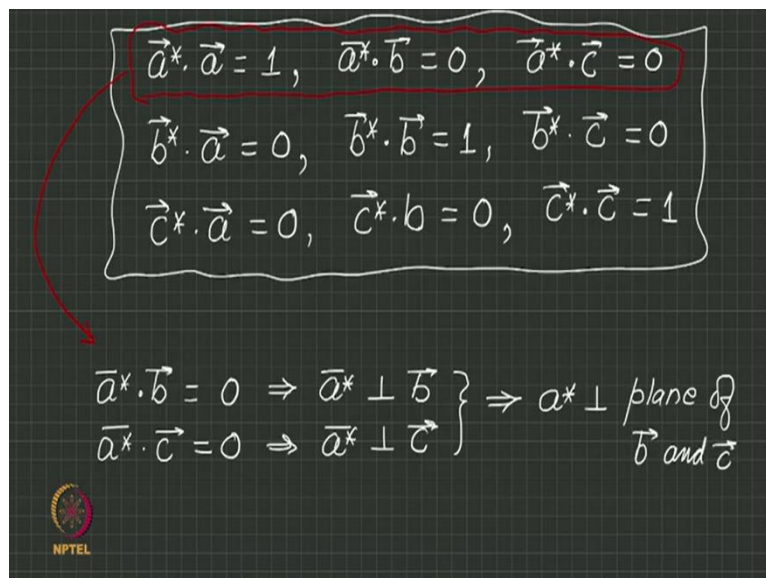
Crystal, Symmetry and Tensors
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Lecture 4b
Reciprocal Basis

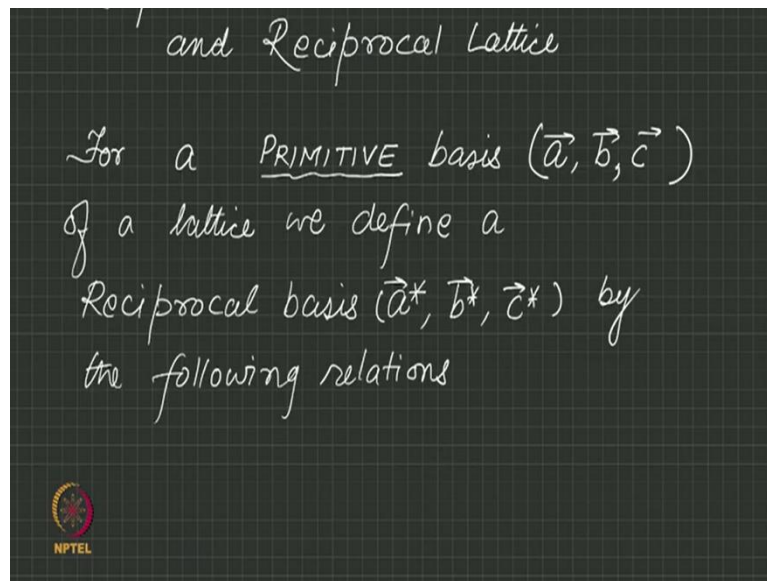
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So, let us now then enter in to our next interesting topic and that is the reciprocal basis. We start with the definition. So, our definition is for a primitive basis abc of a lattice we define a reciprocal basis a star, b star, c star, we are just defining two new three vectors we have a, b and c given to us in terms of those three vectors, I am defining three new vectors a star, b star, c star by the following relation.

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It is very strange and why we are doing it will become gradually clear that yes, it is useful and the beginning at that the point of definition it does not appear to be making any sense. So, what is our defining relations? Our defining relations are actually nine relations nine dot product relations. So, we see $\vec{a}^* \cdot \vec{a}$ is 1 whereas, $\vec{a}^* \cdot \vec{b}$ is 0, $\vec{a}^* \cdot \vec{c}$ is also 0. So, \vec{a} with \vec{a} is 1, \vec{a} with \vec{b} and \vec{a} with \vec{c} will be 0.

Similarly, for \vec{b}^* I write $\vec{b}^* \cdot \vec{a}$, $\vec{b}^* \cdot \vec{a}$ 0, $\vec{b}^* \cdot \vec{b}$ 1 because of same type, $\vec{b}^* \cdot \vec{c}$ 0. Finally, we come to \vec{c}^* , $\vec{c}^* \cdot \vec{a}$ 0, $\vec{c}^* \cdot \vec{b}$ 0, $\vec{c}^* \cdot \vec{c}$ is equal to 1. So, these are the defining relations. So, that is if I am able to find \vec{a} , \vec{b} and \vec{c} were given there was a lattice in that lattice of course, there was infinitely many choice but finally, I made up my mind. With choices in life there is always that issue, once you have more than one choice a lot of time is wasted in deciding which toothpaste to buy so but you have made up your mind and you have chosen \vec{a} , \vec{b} and \vec{c} .

Now, a formula or algorithm is being given to you that if you give me $\vec{a}, \vec{b}, \vec{c}$, I will give you a new metric $\vec{a}^*, \vec{b}^*, \vec{c}^*$ satisfying these relations. So, directly $\vec{a}^*, \vec{b}^*, \vec{c}^*$ is not being given to me, they are being given that $\vec{a}^*, \vec{b}^*, \vec{c}^*$ is such are such that they satisfy these relations. That does not help much. So, let us explore it a little bit more carefully because we want give me \vec{a}^* not the relation which \vec{a}^* should satisfy but give me \vec{a}^* itself. So, how do I find \vec{a}^* ?

So, to find \vec{a}^* let us see which relations are involving \vec{a}^* , the first row. Only the first row had \vec{a}^* in it. The second row has \vec{b}^* and the third row if \vec{c}^* . So, let us explore this one that can we have an explicit formulation for \vec{a}^* using these three relations. So, let

us look at the second relation $\vec{a} \cdot \vec{b} = 0$ because that is a simpler relation, a star dot \vec{b} is 0 dot product is 0, always rings a bell. The two vectors have to be perpendicular.

So at least now I know something about a star that a star is perpendicular to \vec{b} . So, I do not know the full vector. But I know I do not even know its full direction because perpendicular to \vec{b} , perpendicular to a given vector is a whole plane. Perpendicular to my left hand is my current right hand horizontal or now right hand which is vertical. So, perpendicular to a given vector is confining it to a plane but it is not fixing the direction completely, but it is still I know that, if I am being told that it is perpendicular to my left hand, then this cannot be the vector or this cannot be the one. It has to lie in a plane perpendicular to \vec{b} .

So, that is a good information, at least something. If I look at this third relation, a star \vec{c} is equal to 0, then it similarly tells me that a star is perpendicular to \vec{c} . Now I am better off now, I know that it is perpendicular to \vec{b} as well as perpendicular to \vec{c} . So, what does that mean? It is a line which is perpendicular to both \vec{b} and \vec{c} . So, a star is perpendicular to plane of \vec{b} and \vec{c} .

If it is perpendicular to the plane of \vec{b} and \vec{c} from vector algebra, you know, what is the vector which is perpendicular to plane of two vectors? Yeah, $\vec{b} \times \vec{c}$. So, this means that a star is parallel to $\vec{b} \times \vec{c}$ because $\vec{b} \times \vec{c}$ is perpendicular to the plane and \vec{a} is parallel to the plane normal $\vec{b} \times \vec{c}$ is along plane normal. So, a star is parallel to $\vec{b} \times \vec{c}$.

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$$\Rightarrow \lambda (\vec{b} \times \vec{c}) \cdot \vec{a} = 1$$

$$\Rightarrow \lambda = \frac{1}{[\vec{b} \times \vec{c} \cdot \vec{a}]} = \frac{1}{V_p}$$


Volume of the primitive unit cell

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{V_p}$$

$$\vec{b}^* = \frac{\vec{c} \times \vec{a}}{V_p}$$


$$\vec{c}^* = \frac{\vec{a} \times \vec{b}}{V_p}$$

$$\begin{aligned} \vec{a}^* \cdot \vec{a} &= 1, & \vec{a}^* \cdot \vec{b} &= 0, & \vec{a}^* \cdot \vec{c} &= 0 \\ \vec{b}^* \cdot \vec{a} &= 0, & \vec{b}^* \cdot \vec{b} &= 1, & \vec{b}^* \cdot \vec{c} &= 0 \\ \vec{c}^* \cdot \vec{a} &= 0, & \vec{c}^* \cdot \vec{b} &= 0, & \vec{c}^* \cdot \vec{c} &= 1 \end{aligned}$$

$$\left. \begin{aligned} \vec{a}^* \cdot \vec{b} = 0 &\Rightarrow \vec{a}^* \perp \vec{b} \\ \vec{a}^* \cdot \vec{c} = 0 &\Rightarrow \vec{a}^* \perp \vec{c} \end{aligned} \right\} \Rightarrow \vec{a}^* \perp \text{plane of } \vec{b} \text{ and } \vec{c}$$


and Reciprocal Lattice

For a PRIMITIVE basis $(\vec{a}, \vec{b}, \vec{c})$ of a lattice we define a Reciprocal basis $(\vec{a}^*, \vec{b}^*, \vec{c}^*)$ by the following relations



If a vector is parallel to a given vector then what can you tell about its magnitude? Something it will be a scalar multiple. So, but you do not know you do not know what that is scalar multiple is but it has to be some scalar multiple of this where lambda is a scalar. This is very nice. So, but what is this lambda? We have no information about lambda. But recall we have used only two relations given for a star, the very first one we were ignoring till now. So, now, we will use the first one to our rescue and we will be able to find lambda.

So, a star dot a is equal to 1, we did not use this. So, let us use that now and we have a formulation for a star now, as lambda b cross c lambda b cross c dot a is equal to 1 which means lambda is nothing but 1 by b cross c dot a which is called the scalar triple product and what is its geometrical meaning? Again the volume is the same determinant. So, this is 1 by volume of the primitive unit cell remember a, b and c we insisted is primitive. So, this is the volume of the primitive unit cell.

So, we have found λ . So, once we have found λ that means we have found a^* completely now that is $b \times c$ divided by v_p . This was an analysis of the first row, second row involves b^* in a totally symmetric way you can see and the third rows involved c^* in an identical way. So, if you use the same analysis, you will find now that b^* is $c \times a$ by V_p and c^* so, at least we have found our vectors in terms of the original vectors. What they do? We do not know we will find out in the next class that what use we can make of these vectors.