Crystals, Symmetry and Tensors
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Lecture 3a
Plane normal of a plane for cubic crystal

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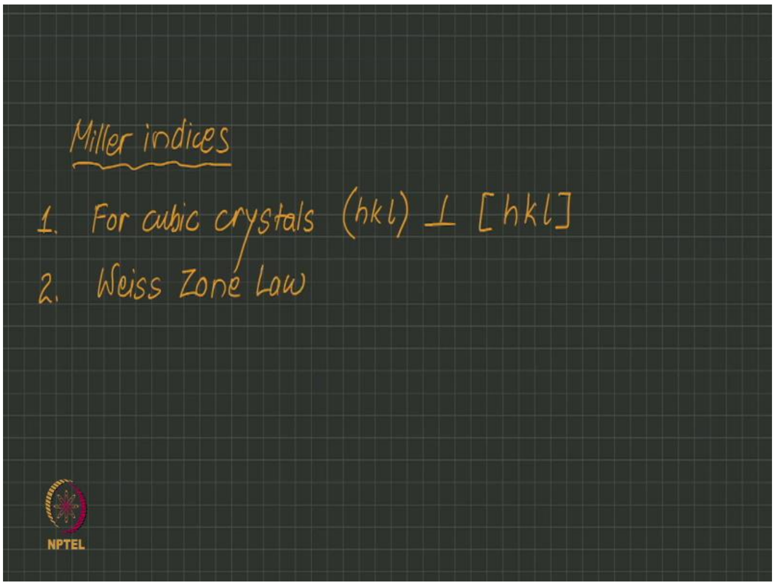

So, welcome everyone, so we have last class we did something on miller indices. So, we will continue our discussion on that. Two important results in miller indices, one is that for cubic crystals, for cubic crystals, see, it is very important to know that plane normal. So, suppose we have a plane hkl. So, we want to know what is the direction which is normal to this plane. Now, for cubic this is very simple, because the plane hkl is always normal to the direction UVW.

So, if direction is given, sorry I made a mistake here, direction hkl itself, direction hkl, so same indices, so nothing can be simpler than that. What is normal to 111 plane? The direction 111. What is a plane which is perpendicular to direction 110? The plane 110. So, they are mutually perpendicular, but we need a proof of that. So, we will give that proof. And the another important result is the Weiss Zone Law which we will see.

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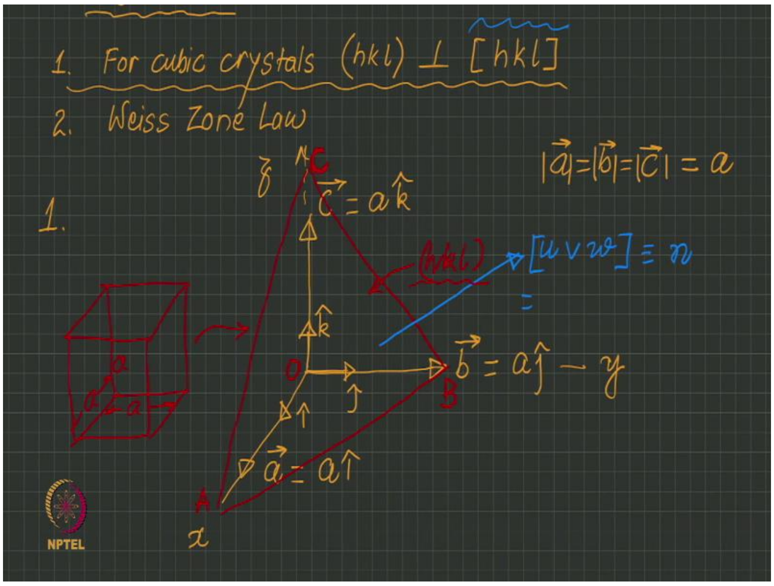

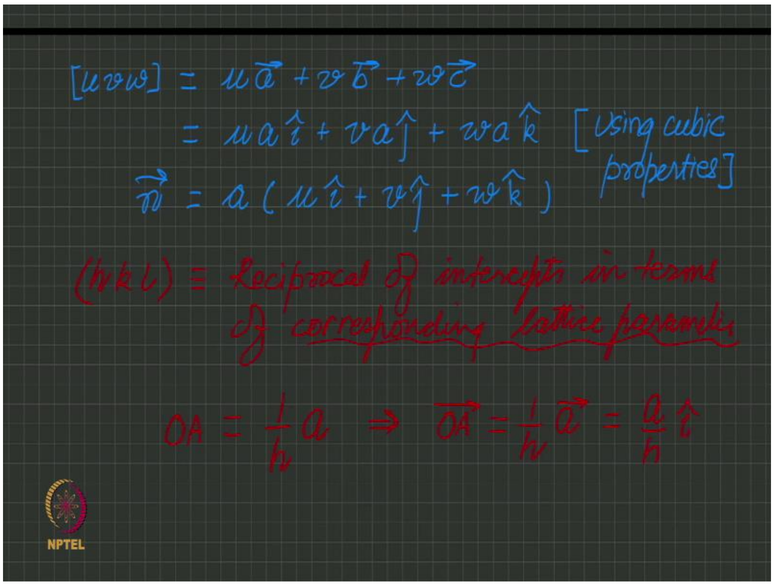

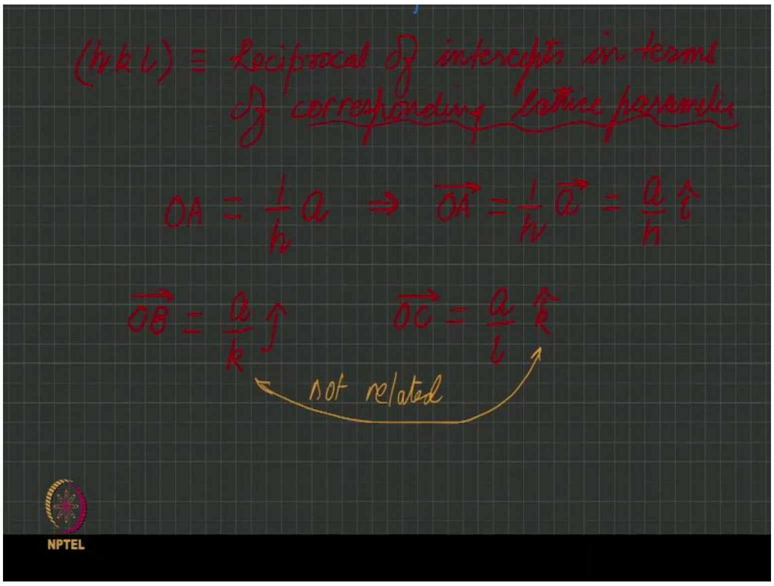

So, let us try to look at these two things. So, first let us prove this property of cubic crystal that the hkl direction is perpendicular to hkl plane. So, let us assume that we have a cubic crystal system. So, in this case the crystal coordinate system is very close to Cartesian coordinate system. Although it is still not Cartesian because crystal coordinate system is still the vectors are of length a, so they are not unit vectors.

So, these are the three-basis vector let us say. So, we know that a, so if we want to write it in terms of the corresponding unit vectors which are let us say i, j and k that is your Cartesian system, then a is simply a times i, b simply a times j. This is a simplicity of cubic that although the vector is b at 90 degree to a but length of that vector is the same as that of the vector in the x direction. So, a, b and c are equal for cubic.

Or, you can say length of vector a, length of vector b and length of vector c all are equal and we are calling that a. So, vector c also becomes a times k. Now, let us introduce our plane. So, let us say that this is our plane. This is the hkl plane. And we are looking for the normal to this plane. So, let us say that this is the normal. And we want to prove that this normal is also hkl direction, but currently we have not proved that.

So, we cannot assume it to be hkl. So, we gave it a general designation uvw. So, that is our, so uvw direction means, in terms of vector, because uvw is the miller indices of the direction and the miller indices of the directions are nothing but components with respect to the crystal basis and the crystal basis is abc, so uvw vector, vector uvw is nothing but u times a plus v times b plus w times c which in the cubic case it reduces to ua times i plus va times j plus wa times k.

So, we have used already the cubic property both of equality of, equality of the three lengths that a, b and c are of equal length, and also, their orthogonality that a is parallel to i, b is parallel to j and c is parallel to k. So, we have used here using cubic properties. For other crystal systems you cannot try this. You will be stuck with ua plus vb plus wc, because a, b, c are not equal, they are not necessarily orthogonal, and so on. So, you cannot write a in terms of i and b in terms of j and so on. So, this is our normal vector.

So, let us give it, this was the miller indices of the normal vector. So, let us say that the normal vector is n. So, this is the vector n. I cannot say that it is a unit vector. So, I am not using hat I am simply using an arrow but I know by assumption I know that this is a vector, which I have assumed to be parallel to my plain hkl. Now, what does the definition of hkl tell you? That is a miller indices of the plane. Yeah, Samyak?

Student Samyak: Second line.

Professor Rajesh Prasad: Here?

Student Samyak: (())(08:19).

Professor Rajesh Prasad: Which one?

Student Samyak: In the second equation (())(08:25).

Professor Rajesh Prasad: Okay, sorry, sorry, sorry, it means, yeah, I was just emphasizing that, that they are equal. I was not saying that they are vector, thank you for indicating that. So, and thank you, thanks for the eraser provided by the notebook I can remove them. So, I was only underlining it while talking. But I was not saying that they are vector, they are scalars. Yes, a is a scalar.

The length of, so we have a cubic unit cell, so maybe I should draw that. So, here, means this is a magnified version where the cube is not shown. And the length, the three edges of the cube are a, a and a. So, that is the lattice parameter, a is the lattice parameter. So, it is a scalar. Now, yes, now, what can you say about hkl? So, what does it hkl plain mean? By the very definition, by the very definition of miller indices, reciprocal of intercepts.

Student: (())(10:09).

Professor Rajesh Prasad: Yes. So, reciprocal of intercepts in terms of corresponding lattice parameters. What do we mean by that? We mean that h, so we mean by, so let us look at the intercepts. So, here is my origin. And let us say oa is the intercept in the x direction, ob is the intercept on the y direction and oc is the intercept in the z direction. So, this means h is representing oa.

So, what exactly that means, that the vector intercept oa I can write as h was reciprocal of the intercept, so reciprocal of h will be the intercept. So, the reciprocal of h will be oa, but in terms of the corresponding lattice parameters, so I have to multiply it by a. So, that will be the magnitude. Or, why complicate the writing we can simply write oa as this.

And which means, if I want to write it in terms of vector I can write it as oa is equal to 1 by h vector a because oa is in the direction of the vector a along the x axis and this will become, in the cubic case, this will further simplify to a by h i because a is ai. By the same token by the same arguments, you can now write ob as a by kj and oc as a by l ijk, a by lk. They are totally different quantities.

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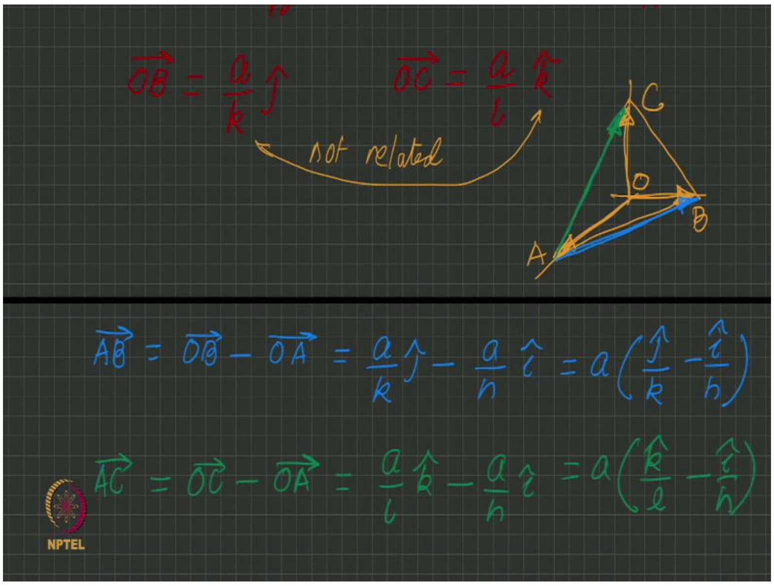


$$\vec{n} \perp \begin{cases} \vec{AB} = \vec{OB} - \vec{OA} = \frac{a}{k}\hat{j} - \frac{a}{h}\hat{i} = a\left(\frac{\hat{j}}{k} - \frac{\hat{i}}{h}\right) \\ \vec{AC} = \vec{OC} - \vec{OA} = \frac{a}{l}\hat{k} - \frac{a}{h}\hat{i} = a\left(\frac{\hat{k}}{l} - \frac{\hat{i}}{h}\right) \end{cases}$$

$$\because \vec{n} \perp \vec{AB} \Rightarrow \vec{n} \cdot \vec{AB} = 0$$

$$\Rightarrow \cancel{a}(u\hat{i} + v\hat{j} + w\hat{k}) \cdot \cancel{a}\left(\frac{\hat{j}}{k} - \frac{\hat{i}}{h}\right) = 0$$

$$\Rightarrow -\frac{u}{h} + \frac{v}{k} = 0$$

$$\Rightarrow \boxed{\frac{u}{h} = \frac{v}{k}} \checkmark \quad (1)$$

$$\vec{n} \cdot \vec{AC} \Rightarrow \vec{n} \cdot \vec{AC} = 0$$

$$\Rightarrow \cancel{a}(u\hat{i} + v\hat{j} + w\hat{k}) \cdot \cancel{a}\left(\frac{\hat{k}}{l} - \frac{\hat{i}}{h}\right) = 0$$

$$-\frac{u}{h} + \frac{w}{l} = 0$$

$$\Rightarrow \boxed{\frac{u}{h} = \frac{w}{l}} \checkmark \quad (2)$$

x

$$[uvw] = u\vec{a} + v\vec{b} + w\vec{c}$$

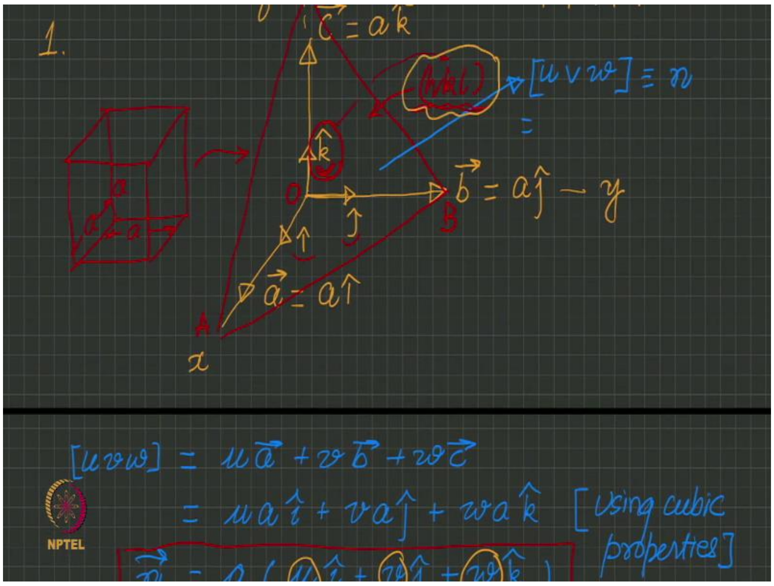
$$= ua\hat{i} + va\hat{j} + wa\hat{k} \quad \text{[Using cubic properties]}$$

$$\boxed{\vec{n} = a(u\hat{i} + v\hat{j} + w\hat{k})}$$

$(hkl) \equiv$ Reciprocal of intercepts in terms of corresponding lattice parameters

$$OA = \frac{1}{h}a \Rightarrow \vec{OA} = \frac{1}{h}\vec{a} = \frac{a}{h}\hat{i}$$

$$\vec{OB} = \frac{a}{\ }\hat{j} \qquad \vec{OC} = \frac{a}{\ }\hat{k}$$



So, now, let us see, let us recall that our plane was like this, our plane was A, B, C and O was the origin and I have developed now formulas for the vector OA, vector OB and vector OC. That means it is easy for me now to write vector AB. Why I am interested in vector AB? Because vector AB lies in the plain, OA, OB and OC are not lying in the plane and I want to explore the plane and I want to find two vectors in the plane.

So, maybe AB and AC appear to be good choices for vector in the plane. So, AB becomes OB minus OA which we have just seen, OB was a by k j minus OA was a by h i. Maybe it would have been better to avoid, means one way of avoiding this k, k interaction could have been to use e1, e2, e3 for the three basis vectors. Then we would have been safe. So, but now we are into it. So, let us not go back and revise that.

Maybe in your notes later on when you are practicing it, you can use e1, e2, e3 in this course also, we accept e1, e2, e3 notation also. So, both are acceptable. So, this is AB, so, we have found one vector in the plane, let us find AC now, the other vector in the plane. So, that OC minus OA, OC was a by l k minus a by h i, k by l minus i by h. Now, I will use this. So, I have, what we have done let us see.

So, we have done a very simple thing that we have found expression for the normal vector, a normal vector n which we had here, yeah here. So, that was simply a ui plus vj plus wk. Please remember that this is u, v and w is what we are unknown, we have assumed and this is what we are trying to find. So, the problem is that hkl is given, hkl is known, we know this is the plane, and I am asking you to give me what is the direction normal to it.

So, we have to find out uvw. So, the goal is to solve for uvw using the fact that the vector n is perpendicular to the plane. And since n is perpendicular to the plane n will be perpendicular to both the direction. So, we can use the dot product condition. So, since n is perpendicular to AB, what do you get? You get a times ui, so, let us write that step also. So, that means n dot AB is 0 which will mean which will give us n was a ui plus vj plus wk.

And a was, AB was a times j dot k minus i dot h. And this is equal to 0 because the two vectors are normal. The plane normal is perpendicular to all the vectors in the plane, so the plane normal is perpendicular to the vector AB. A are scalar, so we can cancel because the other side is 0, so we can divide it by a square. And let us see other vectors. So, we will get, now i j k are orthonormal vectors, so we know that i, sorry, we know that i dot j will be 0, j dot i will be 0 and so on.

So, let us not write all the terms. We know that because of the orthogonality, again these are not to indicate that these are double vectors already they have arrow above them or hats above them. But I was only trying to pinpoint, so, the only terms which will survive is i dot i which is 1 and j dot j which is 1. So, i dot i term is minus u by h i dot i which will come from the first term of the first bracket multiplied by the second of the second bracket.

And then j dot j will come from second term of the first bracket that is v by k. And this is equal to 0. Other terms are anyway 0 when you expand this product out. So, we have u by h is equal to v by k. Now, similarly, you can apply the condition that n is perpendicular to AC, this will give you n dot AC is equal to 0 which is again a ui plus vj plus wk dot a, AC, remember we have found AC k by l minus i by h, k times, k by l minus i by h and this is 0.

Again, i dot i gives you, a can be canceled, i dot i gives you minus u by h again and plus k dot k, so here is k, so you will get w by l, w by l is equal to 0. This gives you u by h is equal to w by l. So, u by h is equal to v by k, u by h is equal to w by l.

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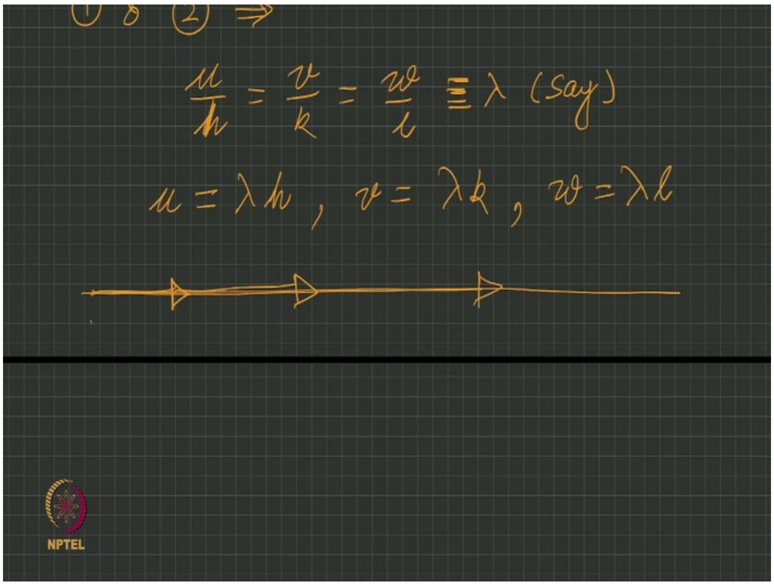

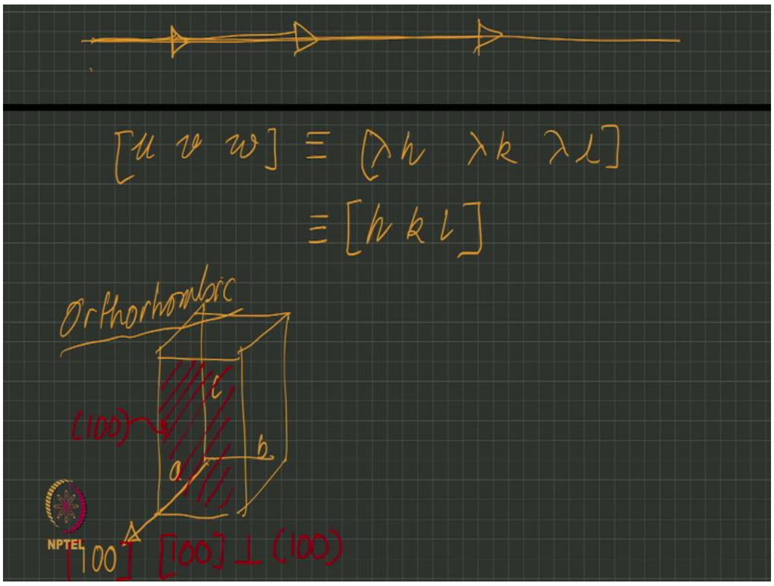

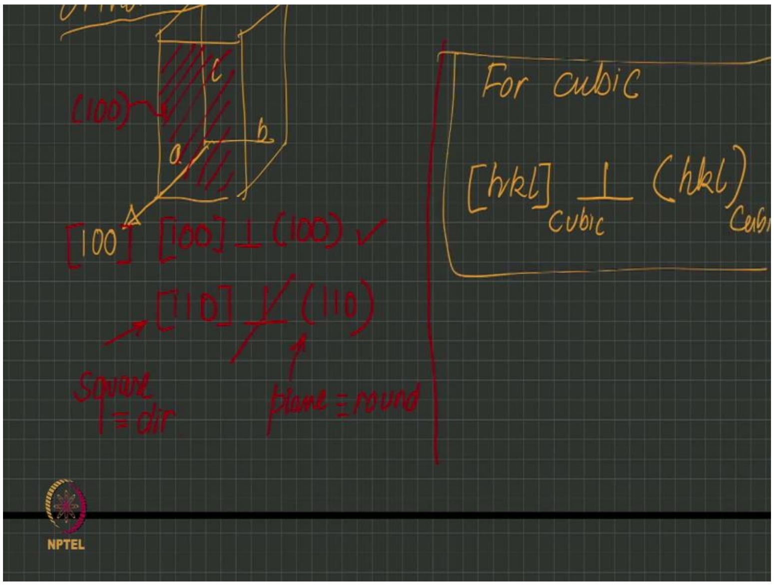

So, from 1 and 2 you can write w by l. And since these are equal ratios, let us say that this equal ratio is something nice to use some fashionable Greek letter lambda, say. We have introduced this is not a quantity which is defined we are now defining it. We are saying that this equal ratio is lambda. So, then u is equal to, because we wanted to solve for u, v and w, so that is why we call it that lambda.

So, u is some lambda times h, lambda times h, v is lambda times k, w is lambda times l. So, essentially, we have solved for uvw except that we do not know lambda. But thankfully in crystallography, you do not have to know lambda if you are trying to find out the miller indices for direction. Remember we said that miller indices have a direction can be defined by any vector because 2 times or 3 times a given vector all will give us the same miller indices.

So, using that property, this lambda actually can be divided. So, we can divide by lambda. So, uvw becomes lambda h, lambda k, lambda l. And dividing by we can say, we have said that, that we can divide by any constant factor, so dividing by lambda we get hkl and that is the beautiful result we were looking for. That is why cubic is so simple. So, uvw becomes hkl. But remember that this is for cubic only.

In some other cases this can still be accidentally true, but you cannot take it for guarantee. So, suppose it was orthorhombic or tetragonal, or orthorhombic let us say, a, b and c are not equal, then along the x axis you have a direction 100. And this face of the crystal is again 100. So, here you are finding that 100 direction in orthorhombic also will be perpendicular to 100 plane, but this is limited to some such a special planes and a especially direction.

Arbitrarily if I, so, if but to, so 100 direction perpendicular to 100 plane in orthorhombic also. But if I say 110 because of the inequality of the a and b 110 will not be perpendicular to 110 plane, 110 direction. And keep remembering if I make mistake you can correct me also and you can always be also alert that whenever we are writing direction we are using a square bracket for direction and whenever we are writing round bracket we are using plain. So, it is not a general result but for cubic it is always true. For cubic hkl direction because we have proved it hkl direction is always perpendicular to hkl plane.