An Introduction to Materials: Nature and Properties (Part 1: Structure of Materials)

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Lecture – 10

Miller Indices (Planes and Directions)

So, this is the start of a new lecture 10, which is which is on Miller Indices Planes and Directions and Crystals. So, in the previous lectures we saw, we understood the fundamentals of crystallography, lattices, crystal systems, revised lattices and symmetry and their correlations. Now, we will try to understand how you can quantify the crystals in terms of the directions and various phases because this is the knowledge of this is very important to understand the correlation of correlation of an isotropic directional response of various properties in crystals as we as you will see as a materials engineer later on in practice that material many of the properties of materials are very and isotropic.

So, if you measure certain property along one direction it is different than other directions. So, and this is true about mechanical properties, it is true about electrical properties, thermal properties and many other magnetic properties.

So, to correlate the properties with directions you need to have a method to quantify the crystals directions and faces and that is where this concept of miller indices comes into picture so.

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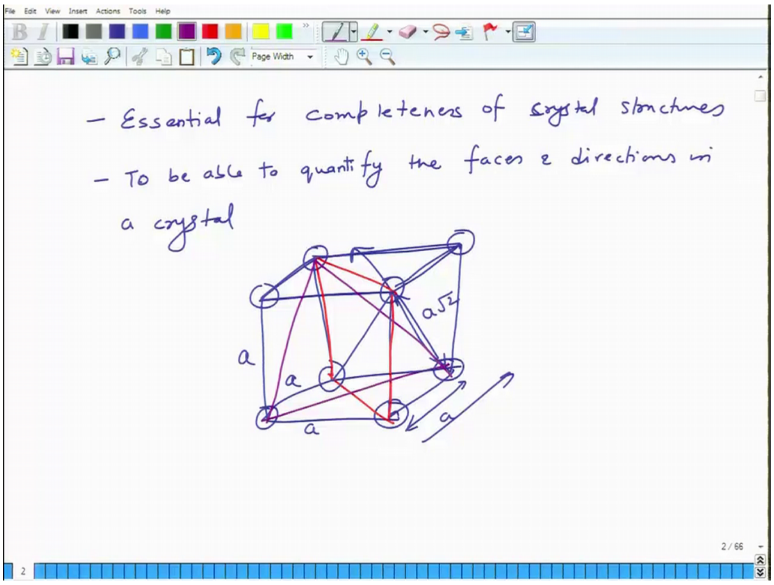

So, basically it is essential for completeness of of crystal structures and to to be able to quantify the faces and directions in a crystal and the reason for that is let us say I draw a simple parallelepiped here so, I have these atoms ok. So, you can see that the separation between so, if it is a cube then you know that this is a this a and this is a you can see that that spacing between these atoms is a, but these atoms is not a, it is something else it is let us say a by root 2 spacing is spacing between this and this is different spacing between for example this and this is different. So, given that different atoms have different spacing's with respect to each other.

The properties also change in different directions. So, if I measure some response in this direction it is different from the response that is measured in this direction ok. So, that is why we need to understand what is this direction, what is this direction, similarly you can see that different faces of crystal has different atomic density for example, this face has these 4 atoms located at certain distances, if I take this face this has a different density it again has same number of atoms, but it has different density. It will change when you go to FCC and BCC structures for example, this face has different density and as a result they will have different response because they have different spacing of atoms between them and there are they are packed differently in these directions. So, that is why it is necessary to evolve a system to quantify these things.

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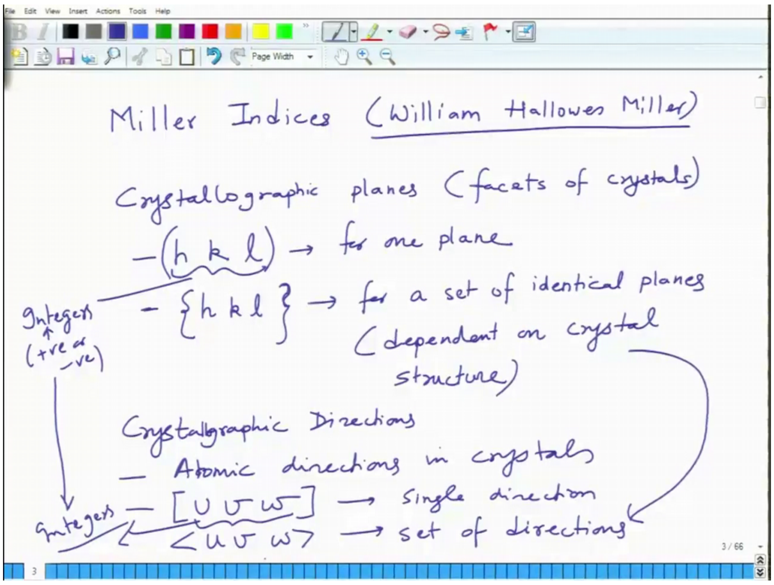

Miller indices are in the name of a person called as William Hallowes Miller who coined the term who depict who came up with the system and that is why these are called as miller indices. For crystallographic planes; planes are nothing, but the faces of facets of crystals you can say facets of crystals they are defined as ah. So, this is to identify they are defined as h k l for one plane in the single bracket and if you have this these brackets they are not applicable to every crystal system, but it could be for a set of identical planes dependent upon one crystal structure whether it is just cubic or whether it is tetragonal. So, you may not be able to write the same connotation for tetragonal if you are able to write the same for cubic.

So, second thing is Crystallographic Directions crystallographic directions are various with various atomic directions. So, you can say atomic directions in crystal and these are depicted as u v and w. So, u v and w in this bracket is a single direction and if you write in this fashion u v w then it is set of directions and again just like planes it is dependent upon the crystal structure and here h k l and u v w all are integers. So, h k l are integers, u v w are integers they can be written there is known there is no restriction on sign, could be positive or negative similarly this could also be positive and negative ok. So, they could be both positive and negative, but they are integers they are not fractions ok.

So, now let us first see the plain thing ok.

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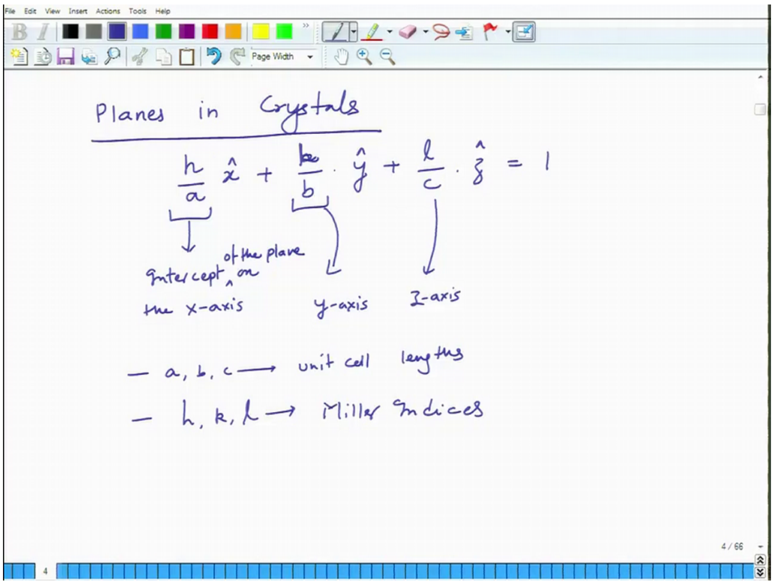

So, this planes in for a plane in a crystal the equation which satisfied the plane in a crystal is h divided by a along x x hat and k divided by b y plus l divided by c to z is equal to 1, where h by a is intercept on the intercept of the plane on of the plane. Similarly, h by b will be intercept on the y axis l by c will be intercept on the z axis and a b c are unit cell lengths or lattice parameters as we call them and h k l are miller indices.

So, let us see following this definition.

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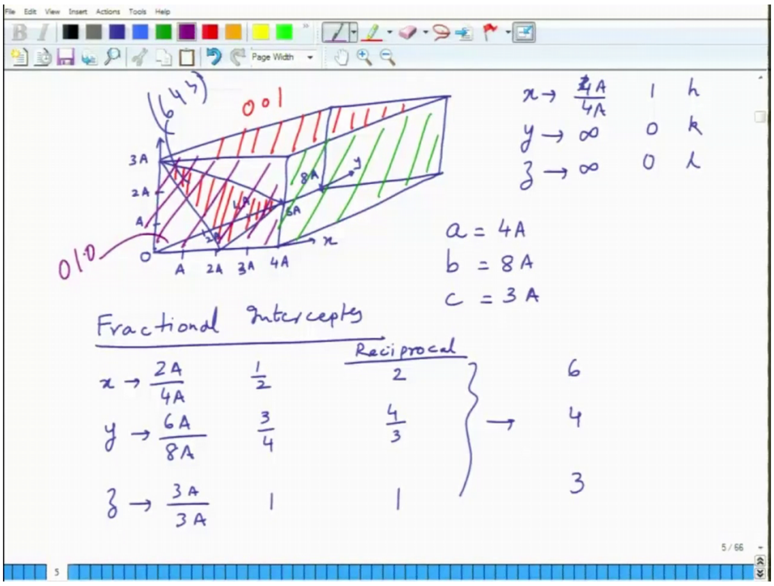

Let us say, I have a parallelogram like this let us say this is the origin and I define this as in some multiple of let us say A, 2A, 3A and 4A here I define as A, 2A and 3A and here it

I define as let us say this is 8A. So, this will be 4A and I have. So, this is 6A and this is 2A. So, I have a body which is something like that and if I connect these so, this is my plane. So, I can see my unit cell parameters are so, a is equal to 4A b is equal to 8A and c is equal to 3A all right. What are the fractional intercepts?

So, fractional intercept along x is 2A by this is along x, y it is 6A divided by 8A and along z it is 3A divided by 3A. So, this is 1 over 2, this is 3 over 4 and this is 1. So, now, you need to convert this into reciprocal so, this is now you take reciprocal. Reciprocal of this is 2, 4 by 3 and this is 1, but h k l has got to be integer ok. So, you need to convert this into a smallest set of integers. So, if you convert this in the smallest set of integers what do you get? You get 6, 4 and 3. So, this plane is 6, 4, 3 that is how you determine the miller indices of a given plane.

So, let us do the same exercise for let us say this plane. So, if you do the same exercise for this plane, now for this what is a fractional coordinate along x fractional interceptor along x? 1, 3A 4A by, what is the fraction intercept along y? Infinity, what is the fraction intercept along z? It is parallel to z, this is z, this is y so, reciprocal is 1 0 0. So, this is h, this is k, this is l, this is 1 0 0 plane likewise if you look at this plane this is parallel to y and x directions, y and x axis, it has intercept of one on z axis. So, this will be 0 0 1. Similarly the one on the front will be this will be 0 1 0. So, this is how you determine the crystallographic plane.

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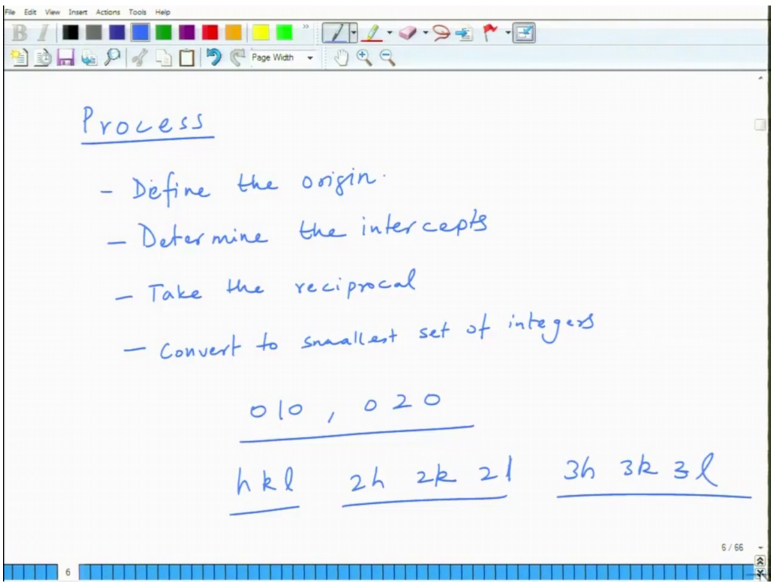

So, basically, the process is the process of determining a plane is you define first a origin calculate the or determine the determine the intercepts, take the reciprocal and then convert to the smallest set of set of integers why smallest set of integers because if you look at 0 1 0 for example, and 0 2 0 these are nothing, but parallel planes one is at the half spacing of the unit cell another is at the full spacing of the unit cell. So, h k l and 2h, 2k, 2l, 3h, 3k, 3l are basically same set of planes they are parallel to each other it is just that the spacing between them is different now ok. So, so this is how you determine the planes. So, if I ask you now to do the reverse exercise let us say.

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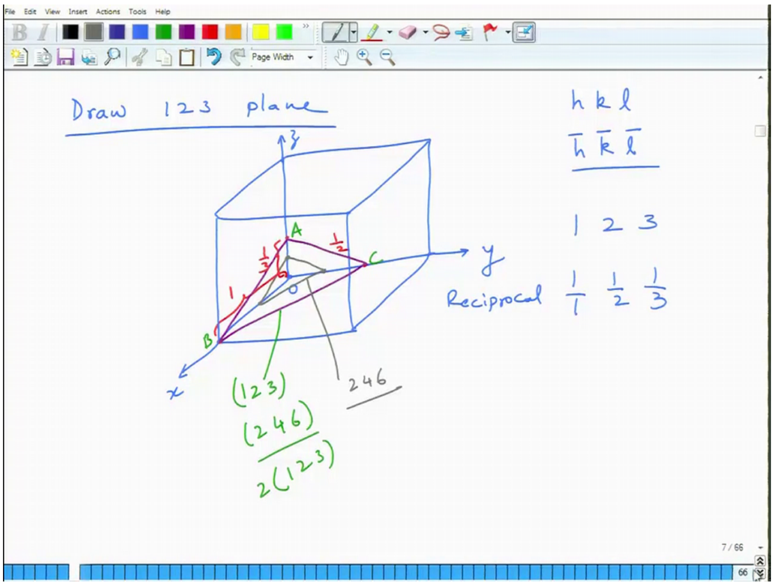

I ask you to draw 1 2 3 plane, I draw a unit cell now here choice of origin is very important how you choose the origin that is very important. Now, let us say conventionally I put this as x direction, this as y and this as positives z, positives x, positive y, positive z. So, I can see that now the key thing about a units key thing about a plane is that a plane has to be drawn within the unit cell itself, it cannot be drawn it should not be drawn outside the unit cell you can draw it, but it is not that is what the purpose the purpose is to draw all the planes within the same unit cell itself..

So, if you have 1 2 3 plane, how do you choose the origin? You can see that h intercept is in positive x direction when you do not have any negative is typically determined as. So, if you have h k l if you have negative sign then it will be bar h bar k bar l ok. So, what it means is that if you have 1, then you are moving you are your intercept is along the positive x direction, 2 means half the intercept is along the positive y direction and 3 means one third of the intercept along positive z direction.

So, the origin which satisfied all the 3 directions is this origin. So, if I choose this as the origin o then my intercept along x axis is 1. So, 1 2 3 should be so, you write 1 2 3 take the reciprocal that is 1 over 1, 1 over 2 and 1 over 3. So, these are the reciprocals and then put them as a intercept in the unit cell.

So, 1 is here, 2 is here and 3 is here. So, this is half this is one third and this is 1 half, one third and 1 is with respect to the lattice parameter. So, it is fraction of so, it is it is it is it is half of the b lattice parameter, one third of the c lattice parameter, 1 time of the or or equal to a lattice parameter 1 means. So, if I now connect these 3 points this we just complete this; this is half ok. So, this is the plane let us say I define as A B C, this is a plane which is called as 1 2 3 plane if you want to draw now let us say. So, just to just to get to you regarding 2 4 and 6 which is nothing, but 2 into 1 2 3 you can see 2 4 6 will be parallel plane ok.

So, 2 4 6 will be half intercept term x, quarter intercept along y and one sixth intercept along z and if you connect these 3 points this will be 2 4 6. So, it is nothing it is nothing, but parallel, but the thing is the every successive 2 4 6 plane will be spaced closer as compared to every successive 1 2 3 plane. So, it is nothing, but family of planes or set of planes which are parallel to each other so, this is about the positive indices.

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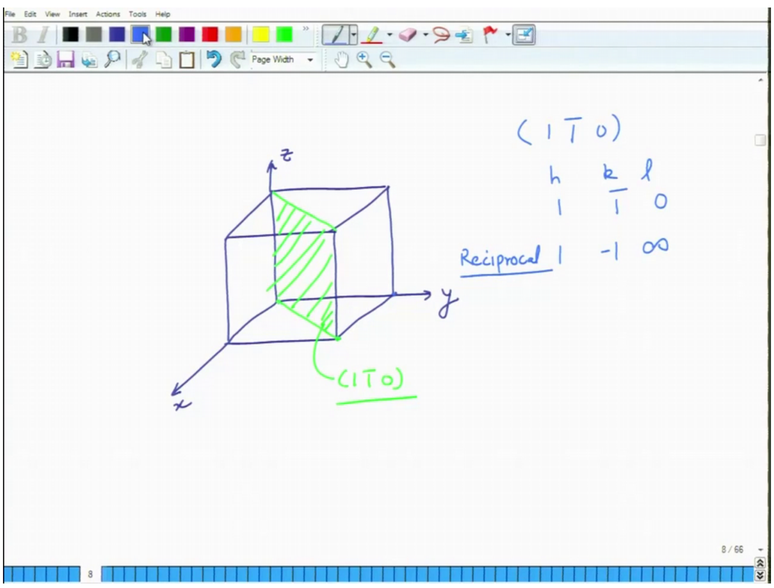

Now, let us say I want to draw a plane which is which has a negative interest indices. So, I draw a unit cell let us say I want to draw 1 bar 1 0 plane ok. So, I can see that h k l is 1 minus 1 0 intercept is 1 minus 1 and infinity reciprocals. So, if I now look at it I have k as minus 1, which means I need to choose an origin. So, that I am able to go minus 1 distance in the y direction. So, if I keep this as the origin I can only go positive in x, positive in y and positive in z; however, if I keep this as an origin if I shift my origin here I can go in positive x and if I go in that direction I go in negative y and this is important to be within the unit cell.

So, if I do that this is the intercept on x, this is the intercept on minus y and there is no intercept on z, which means it is parallel to z right it is infinity. So, the plane would be this and that so, this would be the 1 bar 1 0 plane all right. So, you can do now the exercise at home as to. So, I will just now do one last exercise in this case.

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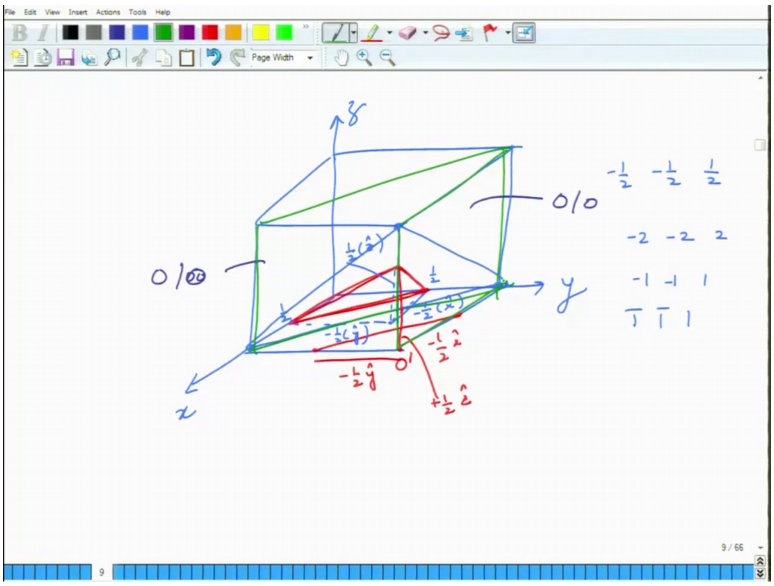

I Draw a unit cell just one last demonstration and just to help you with how to find out the inter in; now let us say I draw a random plane let me choose one. So, I connect this point, this point and this point is it a legitimate plane is it a legitimate plane yes or no you have intercept along x, you have intercept along y and you have intercept along z.

So, how do you choose the origin now? So, you can see that the trick here is let us say so, this is that half right this is that half. So, you can see that if you choose this is this point is located at half of minus half x from here, this is located at minus half of minus half along x, minus half along y and this is at plus along z. So, from this you can work out that this plane is if I look at this minus half minus half and plus half if you take the reciprocal this becomes minus 2, minus 2, plus 2 or this is nothing, but minus 1, minus 1, 1. So, this is nothing, but 1, bar 1, 1..

So, what is 1, bar 1, 1 plane? Basically 1 bar 1 plane will be this and that if I put these together nothing, but a parallel plane, but if you have to determine this red one, this 1 is a legitimate plane as well you might have atom sitting here. So, one way to do it is you do it you do it in this fashion or another way to do it do is could be to draw a parallel plane so that you can choose a origin which is located on one of the corners, which means you have to draw the parallel planes one more parallel plane. So, that instead of ending in this fashion it ends here. So, this will go out of the system ok.

So, basically this line is parallel to that line. So, you can see that if you choose this as a region this is o prime, this is minus half y, this is minus half x and this is plus half. So, this is how you can do so, this line which is somewhere in the in between which is not allowing you to choose the origin draw a parallel line this because these are parallel lines draw a parallel line you can choose now this is the origin, you can change this as a y z intercept, this is a x into y intercept and then come to the same conclusion. So, this is something which is done which you do to determine the planes another thing which you need to know about the planes is the spacing between the planes.

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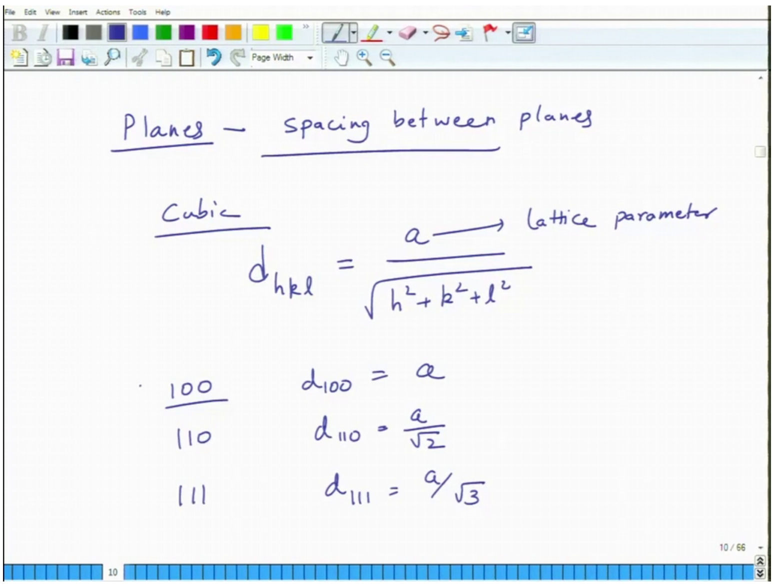

For cubic system spacing between the planes is given as d h k l is given as a divided by square root of h square plus k square plus l square, where a is the lattice parameter and h square plus k square h k l the mirror indices. So, you can see that if you have if I go to the previous ones you have these planes. So, this was one plane this were another plane you will have successive planes. So, what is the spacing between these planes that is or you can have this is 1 0 0 plane, this is also sorry this is 0 1 0 plane, this is also 0 1 0 plane, the spacing between these 2 is a.

So, if you if you put that in so, for. So, for 1 0 0 you will have d 1 0 0 will be equal to a 1 1 0, d 1 1 0 will be equal to a divided by root 2. 1 1 1, d 1 1 1 will be equal to a divided by root 3. So, that is how you can determine the plane spacing and you can also find that different planes are at different angles ok. So, for example, you can see that this is 1 bar 1 1 plane and this is and the. So, you you have you have one plane let me draw a different plane you have one plane which is this plane and you have another plane which is this plane.

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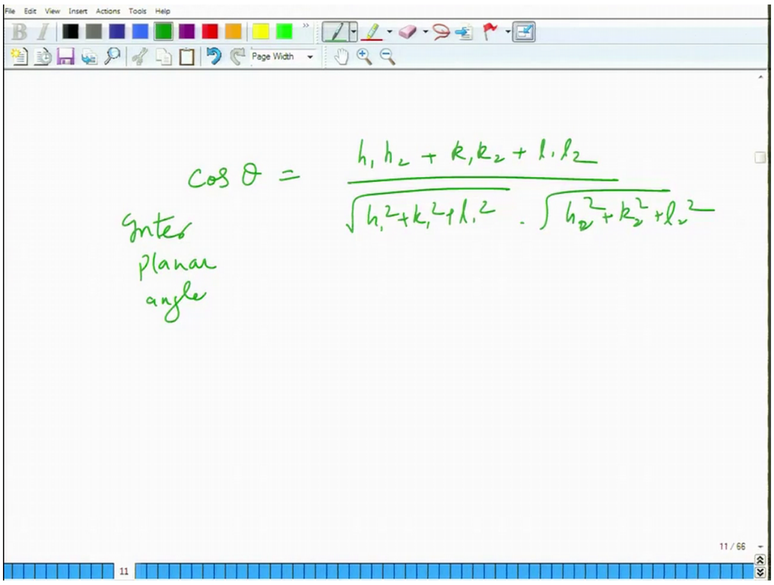

If I want to calculate between the angle the angle between the 2 of them, angle is given as cos theta is equal to h1 h2 plus k1 k2 plus l1 l2 divided by square root of h1 square plus k1 square plus l1 square into h2 square plus k2 square plus this is called as inter planar angle. These are only 4 cubic systems by the way for tetragonal orthorhombic system the relations are different. In the next lecture, we will now discuss the Miller indices for directions so, we will stop here this is only about the planes right now.

Thank you.