X-ray Crystallography

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Lecture - 03
Tutorial 01

Hello everyone. Welcome to this X-Ray crystallography course, offered by professor R K Ray. And I am going to take tutorial classes for all the lecture he has offered. So, the each tutorial will have some set of problems which I am going to solve on the blackboard, which you can use it for solving your subsequent assignment problems. So, what I would like to start is the first chapter geometry of crystals and the second chapter reciprocal lattice. I will solve couple of problems, and then what I request you to do is go through the procedures carefully, and if you have any doubts you can post the questions on the website. And subsequently you must have already seen that the assignment for these first 2 letters has been already posted. So, you can try to solve simultaneously like that.

So, similar manner I will solve all the problems pertaining to all the lectures or chapters, but belong to this course. Then this will basically enable you to solve assignment problems independently and also it be useful to recollect some of the concepts as well as in end semester examinations.

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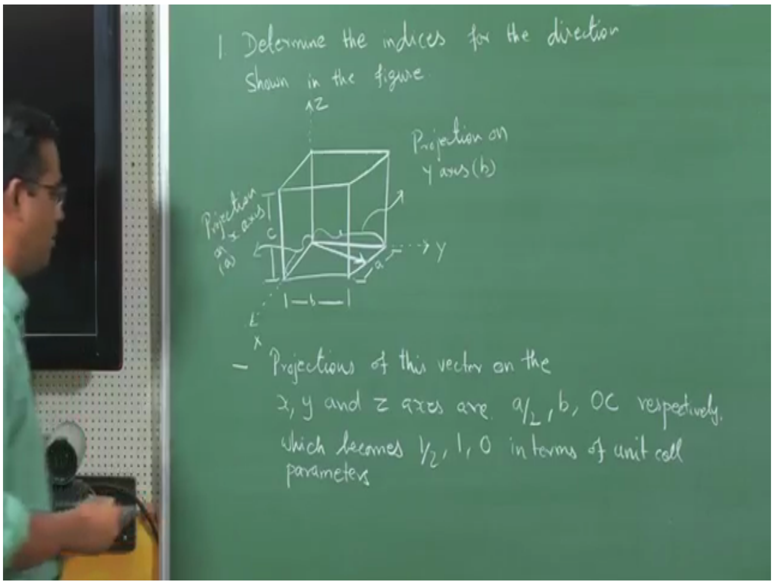

So, let us go to this problems for todays tutorial. So, what I have drawn here is, this is a cubic unit cell and then you have the sides a b and c. And the question is determine the indices for the directions shown in the figure, the this is the direction we are going to determine through the set of procedures you have already seen in the lecture.

So, what you are seeing here is what I have just indicated here is a projection on y axis that is b and this is projection on x axis of a. So, if you can mark like this then it is easy how to move forward. So, what are the steps involved in finding out the direction for this kind of a vector. So, how to go about it? So, there are set of procedure I will just recall. So, what I have done is the first step is look at the projection of this, vector on x y and z axis that is. So, if you see that this is the projection of x that is what I have here projection on y and so on. So, it is aiming to; that means, it is cutting half; that means, a by 2 and then b. So, this is b and then it is c. So, it has gone full length b that is b, but it has come half length in a and then 0 in c. So, this is the first step projections.

And the second step is. So, this, what you have done is which is nothing, but you drop all those a b c then it becomes half 1 0 in terms of unit cell parameters.

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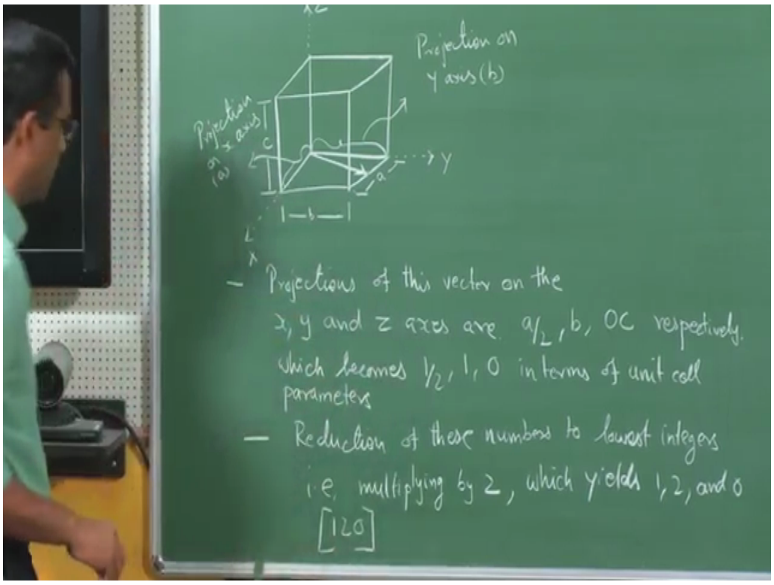

And the next step is you convert that into or reduce into lowest integers that is. So, you have the reduction by multiplying 2 which gives 1 2 0 finally, it can be enclosed in the parenthesis or brackets. So, this is the kind of steps you have to follow.

So, I will repeat the procedures once again. This is the vector we are interested in to find out the direction in this unit cell. So, you take the projection on x y z axis which is a by 2 b and 0 c. Which becomes in terms of unit cell parameters half 1 0, then you reduce this to lowest integers in this case we have to multiply by 2 then it becomes 1 2 and 0 then you put them in the bracket. So, the answer is 1 2 0 that is the correction.

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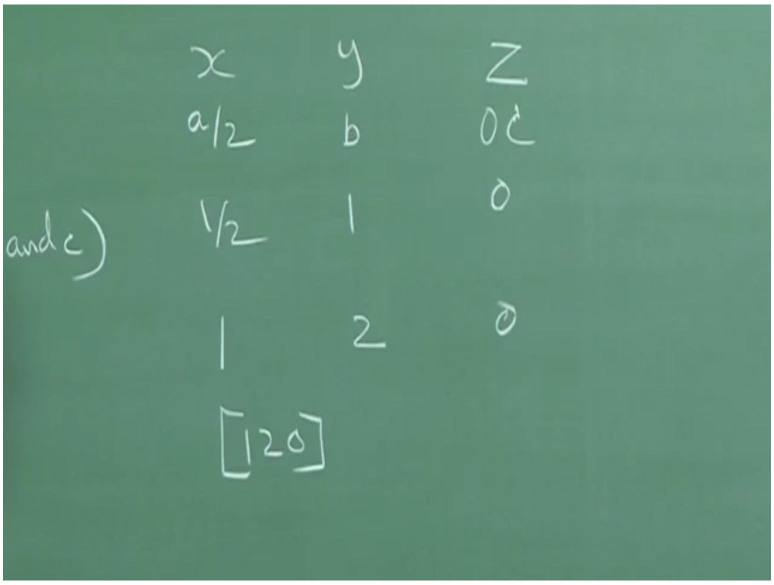

So, probably you can summarise this for a easy you can repeat this for a quick. So, I have put it in the form of simple table. So, you can also create this kind of a table to make it much more simpler. So, this is a by 2 b and 0 c and this becomes half 1 0, this is 1 2 0 direction is 1 2 0. So, you create a table like this for solving any directions a problem like this then it is easy to recapture. So, that is how to go about it. So, let us go to the next problem.

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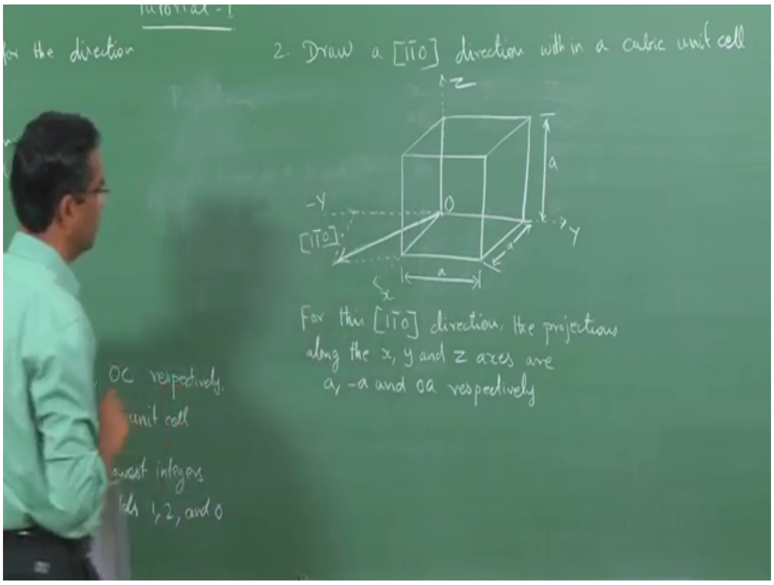

So, it is the reverse what we have earlier seen is we have given the geometry of the crystal and vector and then we have tried to look at these direction. Now you have to draw this direction inside the cubic cell how to go about it. So, this again we will first construct the approximate unit cell. So, since it is a cubic system that will have a similar edge length or unit cell, parameter a let us fix this origin of this unit cell o. So, what we have to do is we have just reverse the procedure what were whatever we have done here. So, we have to come from the bottom. So, we have to find out. So, we have this now 1 bar 1 0. So, for this direction.

So, now we can just start looking at this vector now. So, these are the projections on the x y z axis a minus a and 0 a respectively. So, we have to start from here somehow so; that means, your x is this; that means, this is one towards x you take 1, but why is minus 1. So, this is positive y. So, you have to move into negative. So, this is one and then you start with this. Let us construct this cell again. So, this will be the direction here. So, you move 1 x, and then 1 minus y and then z is 0. So, this will be your 1 bar 1 0 direction. So, this how you should go about it.

So, you should also note that in a cubic unit cell especially you have equivalent directions for example.

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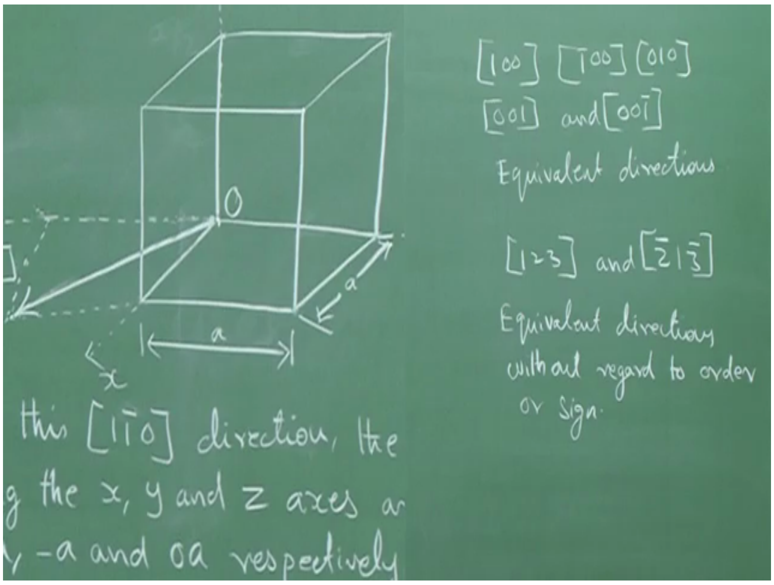

If you know that, they are all equal in directions in a cubic unit cell. So, similarly you can try this for example, 1 2 3 and 2 1 3 or equivalent directions without regard to order or sign. So, this information you have without regard to the order or sign you should know what are the equivalent directions in cubic crystals. So, we will now move on to the next problem that is we will move on to the plane indexing the plane using or finding out the miller indices of a plane in unit cell.

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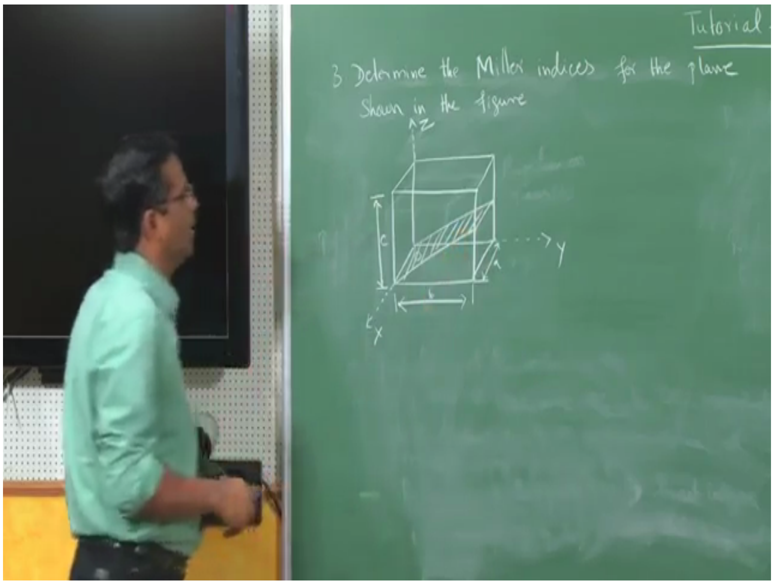

So, determine the miller indices of the plane shown in the figure. So, this is the plane let me shade it. So, I have put a b c need not be a cubic crystal could be a orthorhombic crystal or any excel which is having a different dimensions parameters altogether, but a plane of this kind how do you find the or how do you assign the miller indices. So, you must have gone through the procedures in in the lecture notes.

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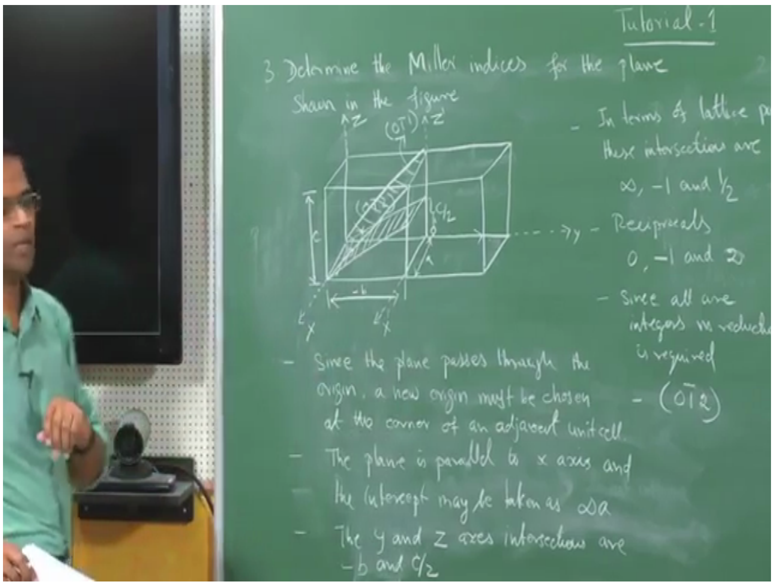

So, how to go about it? So, let us write down the procedures one by one. So, since the plane is passing through the origin that is o here, a new origin must be chosen at the corner of an adjacent unit cell. So, we will do that so. In fact, we can draw a simple diagram again. For I let me put it in the same diagram. So, let me extend this. So, let this be a new origin o dash, and this is z dash x. So, the next point is the plane is parallel.

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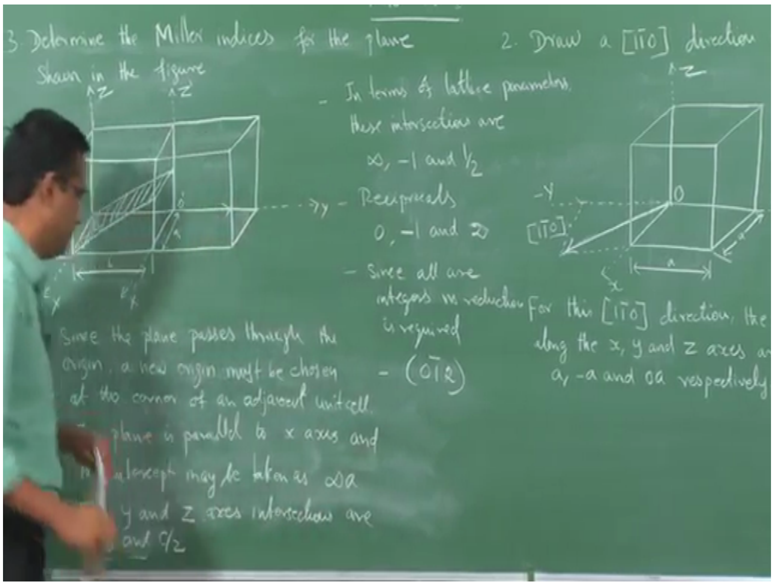

So, what I have just done is we have just come back in the reverse similar manner. Since the plane is passing through the origin we have to extend this to another new origin for the sake of convenience. So, let me mark this intersect also here like c by 2, and this is anyway this is minus b. So, with respect to origin o dash this is minus b, and this is c by 2 since the plane is parallel to x axis the intersect may be taken as infinity a, the y and the z axis intersection are minus b and c by 2. So, you can see that minus b and then c by 2. And this is parallel to x axis the plane is parallel to x axis which is going go on continue like this. So, that is taken as infinity a.

So, in terms of lattice parameters a b c it is infinity minus 1 and half take the reciprocal of this 0 minus 1 and 2. Since these are all already integers you do not have to reduce it further. So, you put it in the parenthesis that is the plane. So, this plane is 0 bar 1 2. So, like that you must have already gone through this lectures and you may find it simple.

So, you practice it for similar plains in different orientations. Then it is easy to arrive at, probably we can look at one more problem. Or let me before even go to the next problem, let me similar to the directions let me summarise this.

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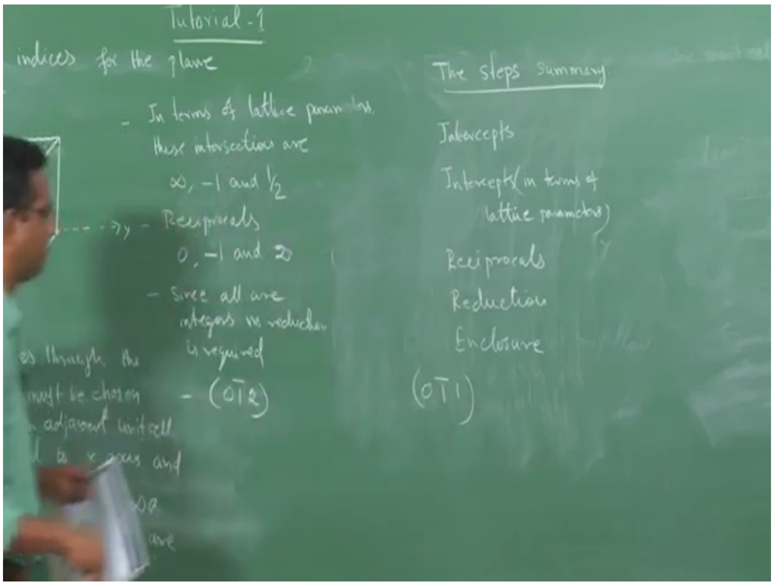

So, the steps summary for finding out the miller indices. First is intercepts in terms of lattice parameters. So, these are all the steps you have to follow find out the intercepts find out the intercepts in terms of lattice parameters take the reciprocals reduce it to a integers and then put it in the enclosure. So, these are all the steps you have to follow for the finding out the miller indices of a plane in a unit cell. So, similarly if you like to try this another similar problem. For example, if you want to try this plane what we have done is 0 bar 1 2. If you want to do this 0 bar 1 1, what will happen is it simply this plane. So, that is 0 bar 1 1. So, basically the c by 2 will become c then this plane is 0 bar 1 1. So, like that you can try some of the other planes as well.

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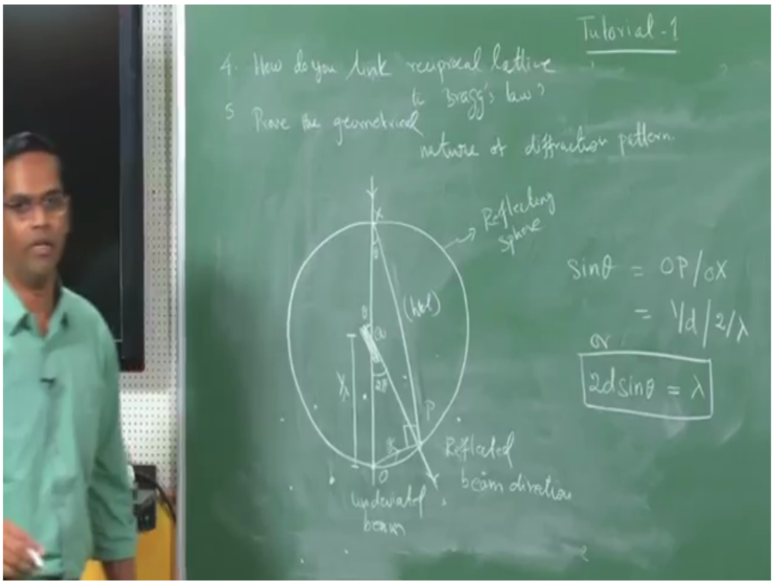

Let me move on to some problems in the reciprocal lattice chapter. So, you have 2 sets of questions for this chapter, as tutorial problems. How do you link reciprocal lattice to Bragg law. So, you know that the concept of reciprocal lattice. And you know what is Bragg law how do you link them. So, that is the question. The other way of putting it is how do you prove a Bragg law using a reflection sphere or evolves sphere. So, you can put it that way as well. So, let me draw the schematic.

So, what I have drawn in this schematic is. So, you have the reciprocal lattice or difraction pattern, which is quite periodic in this in this manner and then I have indicated this is a incoming ray and this is undeviated beam this is reflected beam direction. So, what I have drawn is this is nothing, but reflection sphere or also called evolves sphere. The radius of the evolves sphere as you know is one by lambda. And this is the specimen and then you have the theta this is 2 theta and this is theta this is x, this is o and p and this is the g vector or difraction vector. So, from this what is that we are going to show?

So, if you look at this simple geometrical relation for example, if I write a sin theta of this what will I get sin theta is equal to o p by o x sin theta is o p by o x which is nothing, but one by d divided by o x is 2 by lambda this is one, by lambda this is 2 by lambda. So, o p is this is a g vector g is reciprocal to the d spacing g is equal to 1 by d. So, this is 1 by d by 2 by lambda or you can write 2 d sin theta is equal to lambda. So, what is that we are getting we are getting finally, a Bragg equation. So, what does it indicate so; that means, evolves sphere links, I mean there is a link between a reciprocal lattice that is these points with you know the Bragg law.

So, Bragg law is what the evolves sphere exactly cuts this reciprocal lattice point then it satisfies this condition; that means, when the evolves sphere exactly cut this reciprocal point not ups and down exactly cuts this reciprocal point then this condition is satisfied which is nothing, but a Bragg law.

So; that means, at this condition the di fraction takes place. So, we can say that the evolves sphere or a reflecting sphere link between this reciprocal lattice and a Bragg law. So, this is again indirect way of proving the Bragg law through evolves sphere constructions or you can always say that it is a link between reciprocal lattice and a Bragg law that is evolves sphere construction to it is very simply way of the geometrical construction which always explain the di fraction phenomena in much more explicit manner.

And second thing is let me quickly do that geometrical nature of this di fraction pattern using similar concept what I will do is I will just simply draw the small schematic form there we will take it up.

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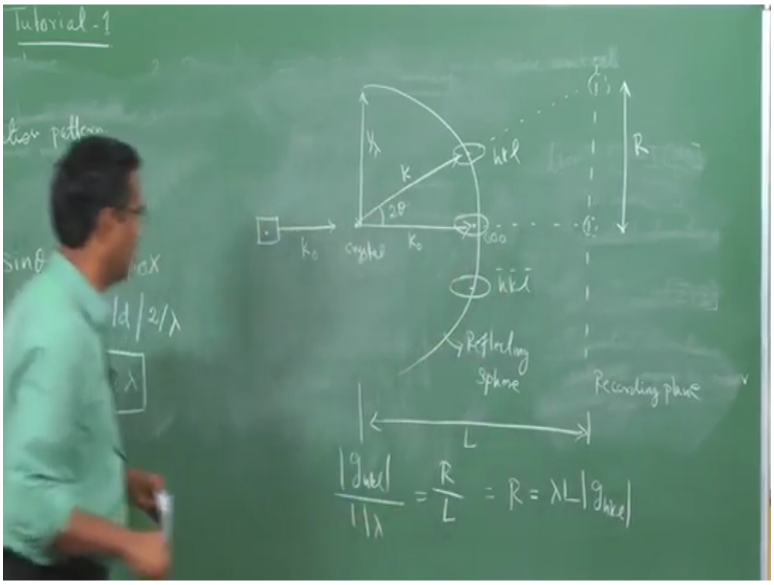

So, what you are seeing here is the geometrical nature of the di fraction pattern. So, you can write this relation g h k l by 1 by lambda is equal to r by l or we can write r is equal to. So, you can use this simple relations to solve some of the problems which we have given in the assignments. So, I would like you to post the questions if you have any doubt then we will take it up in the next tutorial class.

Thank you.