X-ray Crystallography
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Lecture – 06
Tutorial 02

Hello everyone welcome to this tutorial 2. In this tutorial we will look at the assignments problems regarding point groups and face groups as well as the stereographic projections. So, I hope you would have seen in the lecture couple of lectures pertaining to these chapters, detailing the procedures of obtaining a particular stereographic projections as well as talking about a Zonal relationships. So, what we will do today we will just look at suppose if you are given a n number of poles, how to find out the zone axis; which is very simple nevertheless we will just solve some of the problems and then I will just show in a stereographic projection, which I will draw on the board to easily find out how to look at this zone axis pertaining to different poles.

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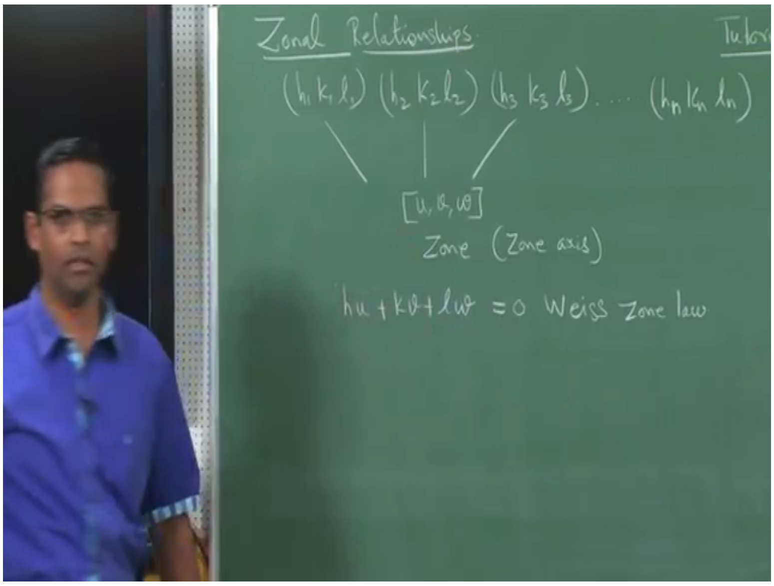

Suppose if I have poles represented by for example, h 1, k 1, l 1, h 2, k 2, l 2, h 3, k 3, l 3 etcetera. So, all of them will belong to a zone called u v w right. In the lectures this is what shown all those zones will belong to I mean all those poles will belong to particular zone. So, you can write something like this, this is zone also called Zone axis and this is called Weiss zone law you will have seen that; let us call it as Zonal relationships. We will now go through general idea about this finding out the zone axis for given number of poles, we will also try to put it in the form of a stereogram.

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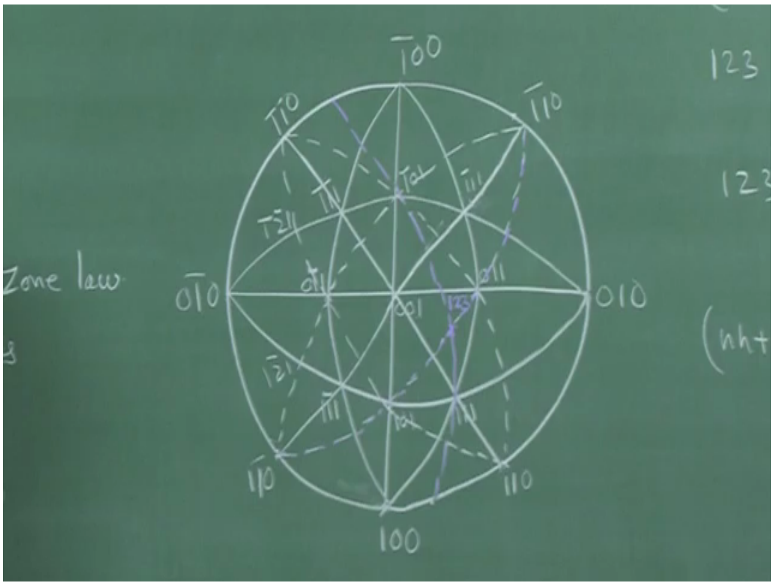

What I am going to do is, which you already know I am going to draw a 0 0 1 projection and them I am trying to find out all the poles which is which can be identified from this stereogram and then we will just look at how this zone law can be directly visualized from this or you can just also try with for a given number of poles how to find out the zone axis.

So, that is what I am going to just demonstrate, which is already clearly and nicely demonstrated in the lecture, but nevertheless if you are given some arbitrary numbers how to go about it with the help of stereogram this is what I am just going to demonstrate in this tutorial class first.

So, what I have drawn here is a standard 0 0 1 projection stereographic projection, and then all the poles I have marked this is a standard one which you all know. So, now, how to find out the Zonal relationship between this 2 according to the. Suppose if you have u b w as a zone axis, then all h 1, k 1, l 1, h 2 k 2 l 2 etcetera, etcetera will be 90 degree towards this pole according to this equation right; these 2 is simply if you consider these as a 2 vector and this is a relationship. So, that is a very simple idea.

So, for example, if you take this 0 1 bar 1 1 as considered as a zone axis, and then you have from the stereographic projection you all know that stereographic projection is the angle through projection, so this from centre to here it is about 90 degree. So, 45 approximately and then you can just have a rough idea about the angle here, then you see that it will be some for this kind of a pole if you see somewhere the 90 degree, you will find this is the great circle and whatever it has falling on this pole will be the corresponding poles of this zone axis. So, similarly you have this zone axis 0 0 1 zone axis, and you have all this poles which is falling on this projection will form a poles. So, this is a zone axis 0 0 1 zone axis and these are all edge pole.

So, if you chose to check whether they obey this Weiss zone law, you take any one of the dot product of this either 0 bar 1 0 dot 0 0 1 will be 0, you take any 1 of these it will obey this law. So, that is the idea of finding out the zone I mean zone axis for a given poles or for a given poles to identify the zone axis, this is the way to do it. You can also identify some of the other important aspects I will just draw few more poles here. So, it becomes little more clumsy, but nevertheless it is a cubic system. Remember 1 in cubic system your all the plane normals are perpendicular to the plane itself, that is a very highly symmetrical nature. So, it is very straight forward to get into this kind of an analysis compared to other crystal systems.

So, you can see that you can simply identify for a given zone what kind of poles will fall into the fall onto the great circle or the vice versa. So, now, I will write some more Zonal relationship.

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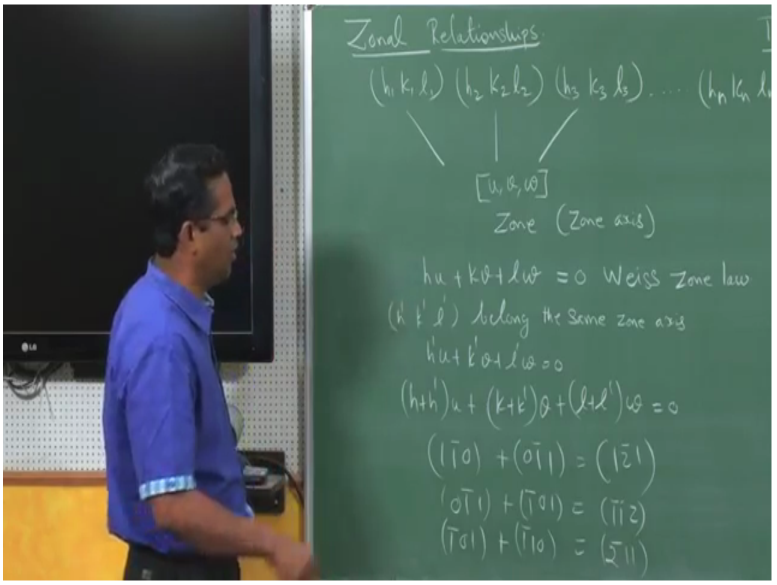

Suppose if you consider h dash, k dash, l dash belong to the same zone axis, suppose if you find some another apart from this some other pole also belong to this zone axis, then that also will follow this rule like I said if you go through this, if you have these kind of relationship also will be valid and you can from this stereogram you can simply look at this kind of relationship. For example, if you add these 2 for example, here 0 1 bar 1, 0 1 bar 1, and 0 bar 1 1, 0 bar 1 0 sorry 0 0 bar 1 1 is here, and 1 1 bar 0 is here. So, if you add these 2 this comes. So, you can check with this also if you even add this 2 the same thing will come.

Similarly, you can find this by adding these 2 or these 2 for example, if you add these 2 bar 1 and 2 bar and 1. So, 1 bar 2 bar 1. So, like that you can keep on generating this pole by this kind of relation. So, since it is highly symmetrical, it is very easy to find out these kind of poles.

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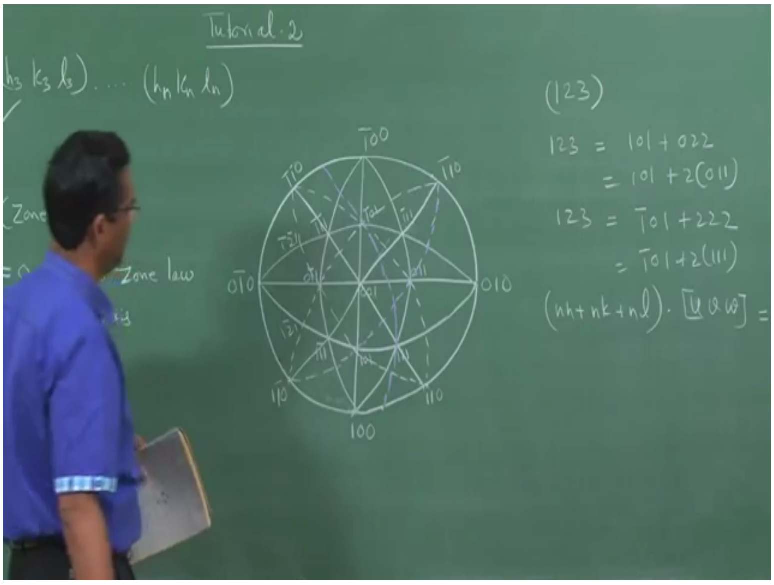

I will just give you one more pecular example, suppose if you have this kind of direction or a pole how to identify this in this stereogram. So, if you look at this you can write 1 2 3 in terms of 1 0 1 plus 0 2 2 which is nothing, but 1 0 1 plus similarly with 1 2 3 can also be written as n h, n k, n l dot u v w is also equal to 0.

So, you see now the simple Zonal relationship we are now extending to its family of directions are playing something like this. So, this you can show it on this stereogram with probably I will take another colour chalk to distinguish already the figure is clumsy. So, to show this 1 2 3 pole what is that you have to do. So, it is combination of 0 1 1 and 1 0 1. So, let us look at this 0 1 0 and 0 1 1. So, we have to draw a great circle which pass through these 2 let us see how it comes, which is nothing but this pole again, which we have already drawn. So, it is easy the other one is bar 1 0 1 plus 1 1 1. So, bar 1 0 1 is here and the 1 1 1 is here. So, we have to connect these 2.

So, now, you see I have connected according to these 2 additions, 2 great circles I have drawn if you look at this intersection which is nothing, but 1 2 3. So, this is how you should visualize this kind of relationship on the stereogram, how to look at this kind of poles which is intersecting on this simple stereogram. So, you have the Zonal relationship. So, this also will fall into these category. So, I think I will I will stop here with the zone axis problem.

So, I hope now all of you will be able to solve this problem if I give you a quite a bit of poles of different sign, you do not have to worry about it simply look at this relation draw a stereogram and wherever you are trying to find the particular zone and its poles which is having this relationship, simply you try to draw this and then find out the corresponding zone axis or the poles vice verse so.

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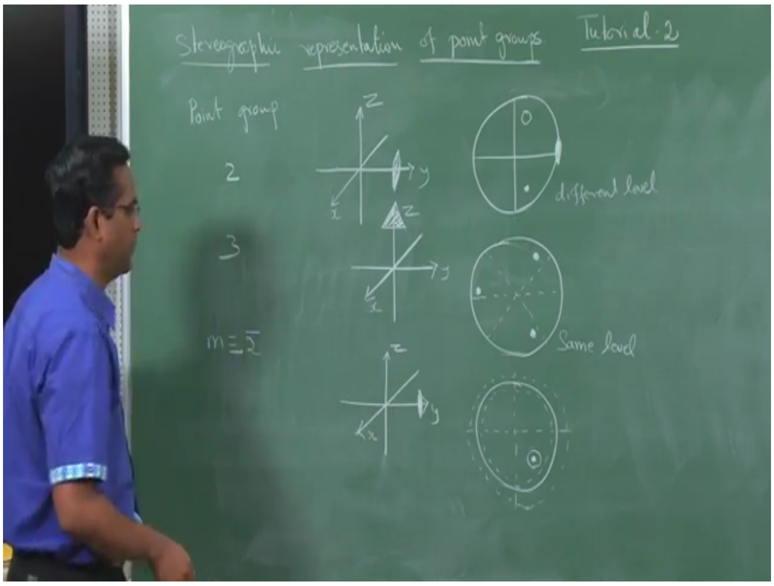

So, next I will move on to some problem on point groups and space groups based on this stereogram. Suppose if I ask you to draw a stereographic representation of point group 2 3 and 2 bar.

So, how to go about it? So, you know that 2 means a rotation. So, you can have a reference like this. So, let me first look at this 2 point group for point group 2, that means, you are having the rotation axis along the y. Suppose this is just shown on the stereographic projection suppose if you have a point here if I do c I mean c 2 that is rotation of 180 degree. If I rotate like this, so it will go to the other end, but at a different level. So, this is on the top and this will go at the bottom if I rotate 180 degree that will go to bottom, but at a different level on at a same level.

Suppose if I have a rotation point group from the top then I will produce equivalent number of positions like this. So, c 3 is 120. So, it will produce equivalent points at these positions, but at the same level. So, what is 2 bar? 2 bar is equal into a mirror, but then still it is 2 bar is rotor inverter. So, that is a symbol 2 bar. So, how to draw this? So, what I have done here is a c 2 with a mirror. So, mirror is when you have a sorry it is a mirror, but it is a rotor inverter. So, what happens when you rotate? So, this will go there it will invert. So, that will come up. So, that is what it is it is all in the same level.

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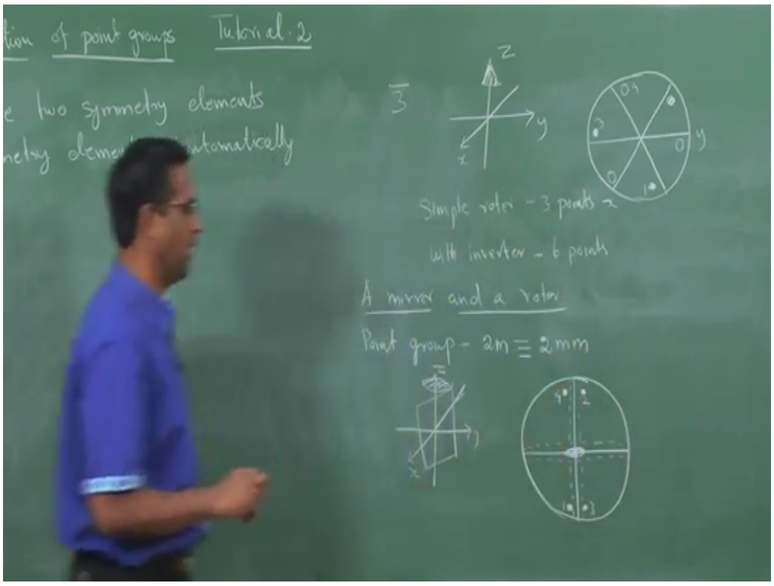

So, you have the mirror which is cutting this plain. Similarly I will show some more examples. So, what I have done here is 3 bar; that means, rotor inverter suppose if I start from this point 1, it will go it is 120 degrees here because it is c three, but it will also invert. So, invert means it has to go through the centre. So, it goes here and 120 invert, again 120 invert, 120 invert 120 inverter.

So, like that it will keep on producing the equivalent points. So, this is at one level this is at the different level. So, you can just follow these kind of notation to follow. So, it will follow that sequence this is for. So, you can say that simple rotor; a simple rotor will produce 3 equivalent points, but with an inverter it will produce 6 points. So, that is the idea you have to remember us go to some little more examples with we will combine a mirror with the rotor for example, the point group 2 m. So, what will happen to this point if you have 2 m; that means, this is a 2 fold rotation in the z axis. So, you have 2 mirrors 1 is here and another mirror is here.

So, what will happen now suppose if I do 180 it will come here, but it will reflect. So, it has to come here right. So, since you have a mirror here this will also reflect here. Since you have then again 180 it will come here, but it will reflect here. So, 2 mirrors this will also reflect here because you have the mirror here. So, a 2 bar m produces 4 equivalent points with the 2 perpendicular mirror here.

I repeat suppose I this my starting point 1 180 reflect, 2 rotation, 3 again this is 4 something like this. So, you just do this it will be obvious. So, you can just try the sequence at a any order you can try, but all that you have to release is this mirror will repeat and this mirror also will repeating it. So, that is a 2 m that is a point of 2 mm sorry 2 m, a combination of rotor plus mirror. So, we can try one more example.

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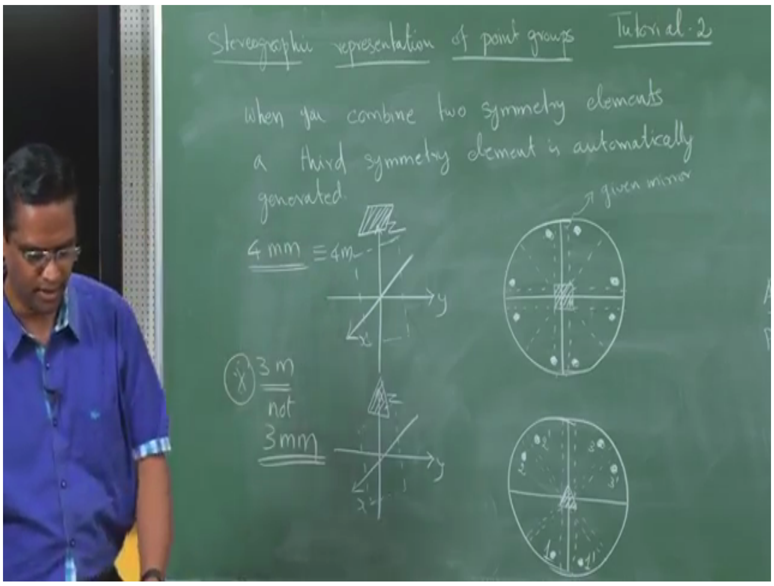

So, what do you find from this kind of a point group this is just a note when you. So, when you combine 2 symmetry elements a third symmetry element is automatically generated. So, that is why it could be also called as 2 mm.

So, we are trying only 2 m, but it produces equivalent positions like 2 mm. So, that is why this sentence. So, let us try now 4 mm point group. So, it will be like this, c 4 rotation axis on the z axis. So, it will produce how many equivalent positions this is just represent c 4. So, I will start with the point here, so 4 mm. So, I will have 2 mirrors. So, when you always combine 2 mirrors it is always considered 2 perpendicular mirrors. So, like you have this. So, if you have this c 4; that means, it will come here it will reflect then it will come here it will reflect, it will come here it will reflect, again it will come here it will reflect anyways this way, it will come here again reflection will come here again reflection, it will come here again reflection.

So, you see that. So, this is given mirror because you have 2 it is 4 mm, but you can see that automatically 2 more mirrors are generated in this how? So, this also a mirror it will also get reflected like this. So, again if combination of 2 symmetry elements, produces other symmetry automatically this is one of the examples of that nature. So, like this we can keep on solving several problems, what I would like to do is you try a different different combinations of this simple rotation to simple mirror, then inverter, then combination of rotation inversion rotor inverter and then rotation plus mirror. So, like that you yourself can combine several point groups and then try to project it on the stereogram like this, and then see how many equivalent points will generate. So, that will be a good exercise, this also will be this kind of exercise also will be used very useful to realize the symmetry in the crystal structures and so on.

So, probably I will solve one more problem then we will stop. So, this is the c 3 axis and you have the mirror along z direction. So, you see here is slightly different from what you have 4 m or which is here it is not the case, here you see you have this 120, since you have mirror here it will have reflection again 120 this you have mirror here it will reflect. So, like that this mirror produces 6 equivalent points, but you can also realize that it generates 2 more mirrors here. So, it is when you say 4 m is equal to 4 mm, you cannot say here it same here because it is not producing a perpendicular mirror plain, but there is an angle between the mirror.

So, you can say that 3 mm is not 3 mm. So, this is very important 3 m is not equivalent to 3 mm, but on the other hand you have 4 mm is 4 m, 2 m is equal to 2 mm, since it is not producing 2 perpendicular mirror in this operation. So, I will repeat you produce this, the first point rotation and there is a mirror. So, reflection rotation there is a mirror reflection, rotation mirror reflection. So, this things keep on generating this 6 equivalent points for 3 m. I think we can one keep on going ahead with this kind of several explanation or similar point group space group exercise through stereographic representations.

So, I want all of you to try similar exercises and then get back to me if you have any doubt and you can post your query or doubt. I hope these exercise will be useful in solving some of the assignment problems which we will post.

Thank you all.