Chemical Crystallography
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Theoretical Understanding of Crystal Packing and X-Ray Diffraction in Direct and Reciprocal Space
Lecture – 21
Tutorial - 3

Welcome back to the course of Chemical Crystallography. Today, we will have a Tutorial on the topics that was discussed in last few lectures.

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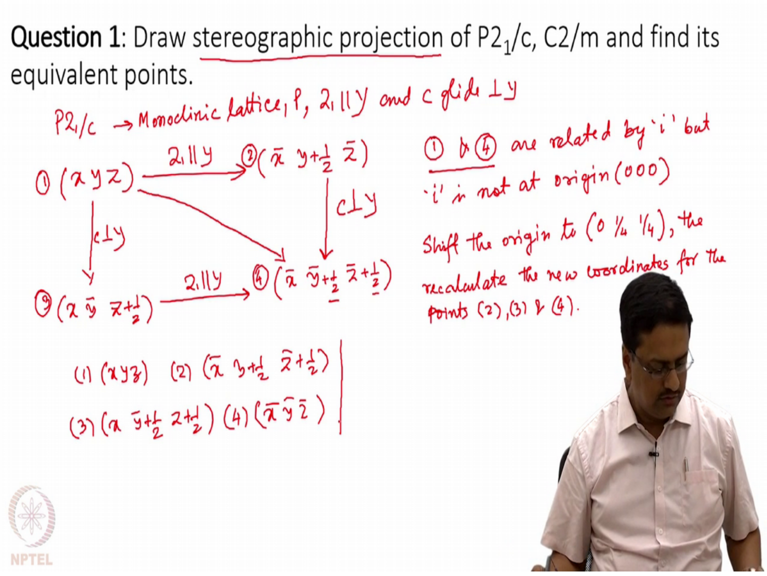

This is based on the assignment that was given to you on third week. So, this is the discussion on the problems that were that was given in the assignment in week 3. So, the first problem that you can see here it is asking you to draw the stereographic projection of P 2 1 by c, and C 2 by m and to find the equivalent points. I hope you understood how to do this, and we will try to work it out quickly for these two space groups.

So, let us first start with P 2 1 by c. So, what is this, this is a space group in monoclinic system right. And it is a primitive lattice. It has a symmetry 2 1 parallel to y and a c glide perpendicular to y. So, if we just try to get the equivalent points by starting from x y z, if we simply apply a 2 1 screw parallel to y, we should get x bar y plus half of z bar.

We apply the c glide perpendicular to y on x y z, what we get is x y bar z plus half. So, now, if we apply 2 1 parallel to y on this point number 3, if we name number them as 1, 2, 3, and the 4th point that we get is nothing but x bar y bar plus half z bar plus half. Remember that when we are doing 2 1 parallel to y, it is x is becoming minus, y we are adding half, because the translation is along y; and z bar it is here it would have been minus z minus half we convert that minus half to plus half by adding one unit along z so that has already been incorporated here.

So, now, what is the relationship between the point 2 and 4, this is again, c glide perpendicular to y. So, now if we look at the points 1 and 4, they are related by an inversion center i, but i is not at origin that is it is not at 0 0 0. So, this i not being at origin indicates that the origin has to be shifted at some point, where should we shift the origin, we need to look at these two points, and see that there is a component of half translation along y and z which prevents these two points from becoming inversion related at origin.

So, we shift the origin to a new point 0 one-fourth, and then we should recalculate the new for the points 2, 3 and 4. How this transfer transformation has to be done I have shown it in the class for 2 1 by m space group. So, you do it yourself in the same manner. And if you do it right, what you would get are the points which are like this. The first point is always x y z; point number 2 is x bar y plus half z bar plus half; point number 3 as x y bar plus half z plus half; and the 4th point is x bar y bar z bar.

Now, with the stereographic projection that means, how these symmetry elements are represented in a two-dimensional pattern is this stereographic projection, and we have discussed this in the class. So, I am not going to elaborate it here. There are different sources where you can get these images I am check your answers. In case, you have any difficulty you can write back to me. Now, let us see what happens when it is a different space group C 2 by m.

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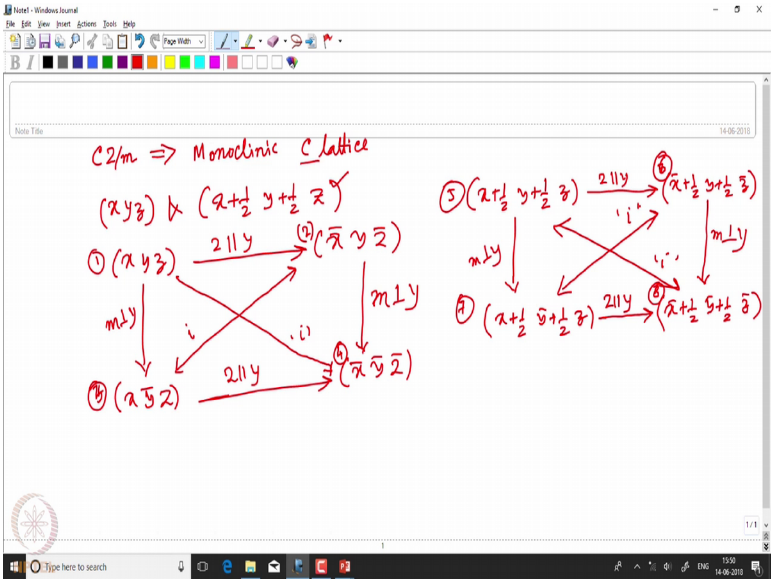

So, when we have a space group like this, it means it is a monoclinic c lattice which immediately indicates that you should have points x y z and x plus half, y plus half and z as equivalent points because of C centering. So, what we should now do is apply the symmetries on both x y z. So, we apply 2 parallel to y, you should get x bar y z bar; we applied m perpendicular to y, we get x y bar z; you again apply 2 parallel to y you would get x bar, y bar, z bar.

And then if we have to try to relate, it is again mirror perpendicular to y. So, here we get 4 points from the original point x y z. The relationship between point number 1 and 4 is i relationship between sorry 2 and 3 is also i. So, there is no need for origin shift in this case the inversion center coincides with the origin.

Now we start with this fourth point; which is fifth point; which is x plus half y plus half z. We do a two-fold parallel to y. We should get x bar plus half, y plus half, z bar. If we do a mirror perpendicular to y on point number 5, we get point number this is point 6, this is point number 7, which we get as x plus half, y bar plus half z. Remember again here when we are doing mirror perpendicular to y, this means it is becoming minus y minus half, we are adding 1, along y to make it y bar plus half and z. Then we apply again 2 parallel to y, you should get x bar plus half, y plus half, sorry y bar plus half z bar.

So now this 7 and 8 6, and 8 are related by mirror perpendicular to y so, once again we see that the points 5 and 6 are inversion related similarly 6 and 5 and 8 are inversion related 6 and 7 are inversion related. And we do not need to do any origin shift for the stereographic projection once again I want you to look at the textbook and get the drawing are here yourself.

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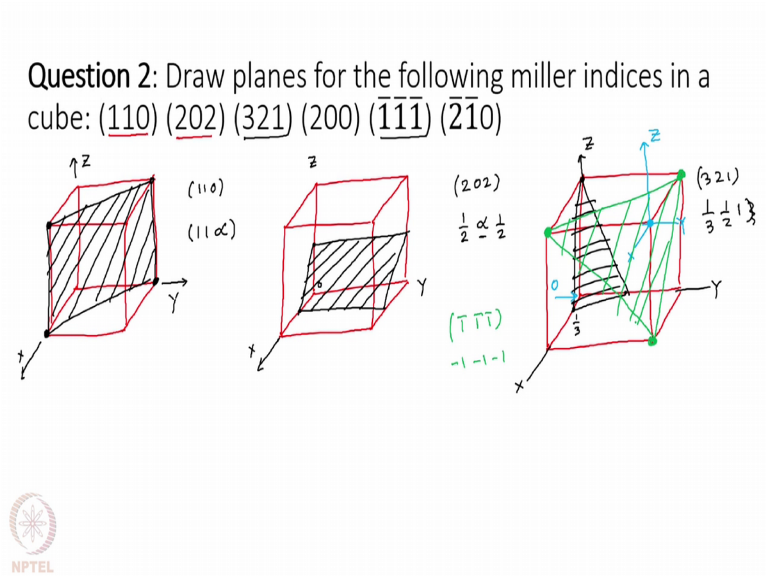

So the next problem which we had here in this assignment, the question number 2. Here you are supposed to draw a few h k l planes with given designations inside a cube. So, the first one is 1 1 0 plane. So, first we should draw a cube. And what we note here, when it is 1 1 0, the plane is 1 1 0 that means the intercepts should be 1 1 infinity which means this plane this parallel to z.

So, if we assume x in this direction, y here and z up, the intercept on x is 1 intercept on y is 1, so this means the plane is like this. So, this is the 1 1 0 plane in the unit cell. The next one is 2 0 2 one second we should draw a cube, and then try to find out the intercepts.

So, the plane is 2 0 2 which means the intercepts should be half infinity half, so when we have infinity as intercept in h a sorry in k it means that the plane is parallel to y. So, now if we start at origin the x intercept is half z intercept is half. So, the x intercept half means the plane should be something like this; is that clear.

The next plane that I want to draw is the 3 2 1 right. The 3 2 1 plane inside the lattice is going to be little difficult to imagine when we say 3 2 1 the intercepts of one- third half 1, so if we assume this direction as x y and z as before the intercept on x axis is one-third somewhere here intercept on y axis is half, so the intercept is here, and intercept on z axis is 1, so it meets there. So, the plane is like that.

Now, I want to draw this 1 1 1 plane in this same cube. So, this is not 1 1 1 this is 1 bar 1 bar 1 bar. So, this 1 bar 1 bar 1 bar plane indicates that all the intercepts are negative. So, if we consider the original origin as origin, then it will not be possible to draw insides the cube. So, to draw it inside the cube we need to choose a new origin such that all the intercepts will be negative so, to do that we choose the other diagonally opposite point as the origin, and make it x, y and z in this direction.

So, now the intercepts are going to be if the plane is 1 bar 1 bar 1 bar, the intercepts are going to be minus 1, minus 1, minus 1. So, with respect to this new origin, the minus 1 along x is there, minus 1 along y is here, and minus 1 along z is at that point. So, we are talking about the plane which is this one right. So, I leave it to you have to draw the other two planes.

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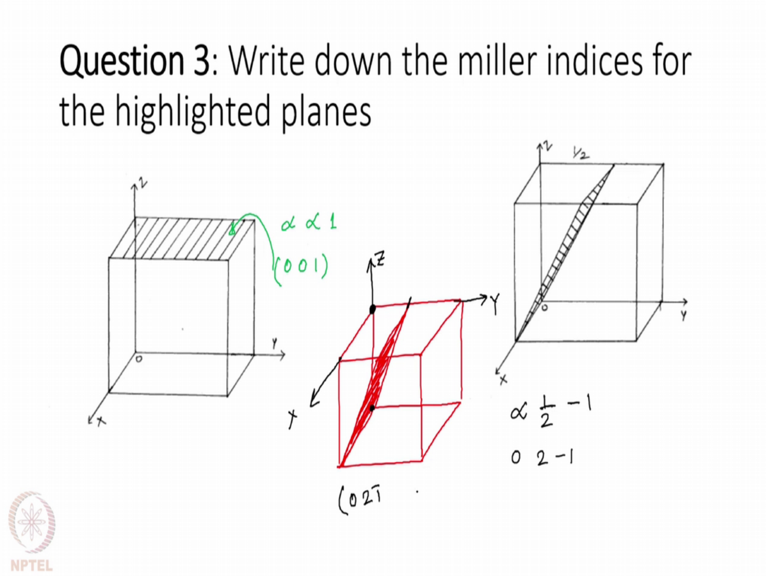

The next point where we have the question is you have to identify, and to identify the Miller indices of some of these planes. So, let us see the first one here the first one as you could see is parallel to both x and y, because it is having x and y parallel. So, intercepts along x and y are infinity and infinity, and it cuts z at 1, so you take the reciprocal 0 0 1 and, then enclose it in the first bracket, so this plane is 0 0 1 plane.

Now, you see we have given another plane this particular drawing is not very clear, but what I want to show here is that we mean to get the Miller indices of this plane. So, what it means that this plane is passing through the origin O. So, once a plane is passing through origin O, we must shift the origin to a desired suitable position. So, if we now shift the origin to this point, and consider the plus direction of x here, y and z so now we can see that this particular plane is parallel to my x axis. So, the intercept along x is infinity this plane meets y at half and it meets z at minus 1. So, if we take the reciprocal of that, it becomes 0 2 minus 1. So, this particular plane the Miller indices would be 0 to 1 bar.

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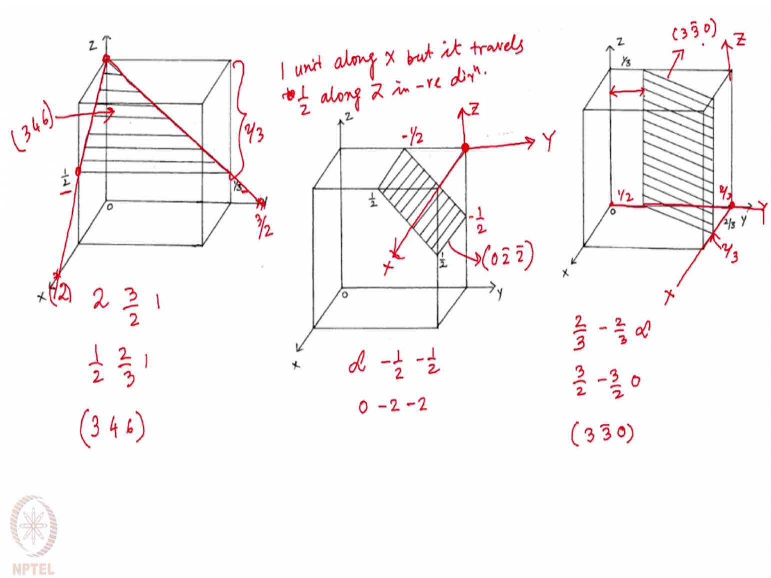

Now, if we look at this particular plane, what we see here is that the intercepts that are given are both given along z. This one is half along z, this is one-third along z which means that the particular line which is coming from z equal to 1 like this has to go and meet y at some point. And similarly the other line which comes like this has to come and meet x at some point.

So, what we see that the line from here to there come travels, 1 unit along the lattice or along x, but it travels half along z in negative direction. So, this point this line would meet x axis at 2. Similarly, this line has travelled one unit along y, while it has come down by two-third along z. So, to get down by another one-third, it would go and touch here at 3 by 2. So, the x intercept is 2, y intercept is 3 by 2, and z intercept is 1. So, you take the reciprocal half, two-third, 1, clear the fractions 3, 4, 6. And this is the Miller indices of that particular plane which is drawn here.

The second next plane which is given looks like that. Once again what you should notice is that if we consider origin at the given point, it becomes difficult to visualize the intercepts. So, we should shift the origin to a convenient, location we can shift the origin to this point and consider this direction as x y and z. So, now with respect to the new origin, this plane is parallel to x, so the x intercept is infinity it meets y at minus half, and it meets z at minus half inning. So, by taking the reciprocal, we get 0 minus 2, minus 2. So, this is the plane having indices 0 2 bar, 2 bar. The next plane which is there is also required that we shift the origin to a new place.

Because, with this origin which is marked in the figure, it is difficult to visualize the intercepts we shift the origin to a new position here and consider this as x, y and z. So, now, with this new origin, we see that this plane meets the x axis at two-third; y-axis it meets at minus two-third, because this one-third is measured from the old origin, so this is one-third. So, the remaining portion that side is two-third, so it is from that origin it is minus two-third and it is parallel to z as we can see. So, the z intercept is infinity. So, we take the reciprocal so 3 by 2 minus 3 by 2 0.

So, we now clear the fraction, and write it as 3 3 bar 0. So, the Miller indices for that is 3 3 bar 0. So, today we have discussed about the Miller indices, how to draw the planes inside and cube or when a cube is drawn how to determine the miller indices of a plane. So, in the next class, we will continue discussing these and then in the following tutorial we will solve some more problems.