Chemical Crystallography
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Basics, Symmetry and Equivalent Points in Crystallography
Lecture - 04
Equivalent Points and 1D Lattices

So, in the previous class we were discussing about the Crystallographic Symmetry and their Notations. We discussed how one should represent 2 fold, 3 fold, 2 bar, 3 bar etcetera 4 1, 4 2 different types of screw axis. And then we discussed about how the glide planes are to be drawn on plain paper and if you are studying a book were these drawings are made you should be able to understand what kind of symmetry elements it represents.

So, now I would like to take you through the symmetry elements and the corresponding equivalent points that are drawn in three-dimension. See what are equivalent points? In crystal lattice there will be one molecule at some place and there will be other molecules in the lattice related to the original molecule through a particular symmetry. A molecule can have a mirror symmetry, a molecule can have a 2 fold rotational symmetry, a molecule can have a 3 fold symmetry, not the molecule the crystal structure may have a 3 fold symmetry. So, that one molecule is related to other one by 3 fold.

So, the starting point is called the original point x y z and then you apply those symmetry elements on x y z and generate new coordinates at different places in the lattice and that those extra new fully generated points are called the equivalent points. So, in three-dimension when we try to generate these equivalent points what we need to do is to apply the same concept that we discussed in the previous class that in two-dimension, but now we will see what happens when we apply that in 3D.

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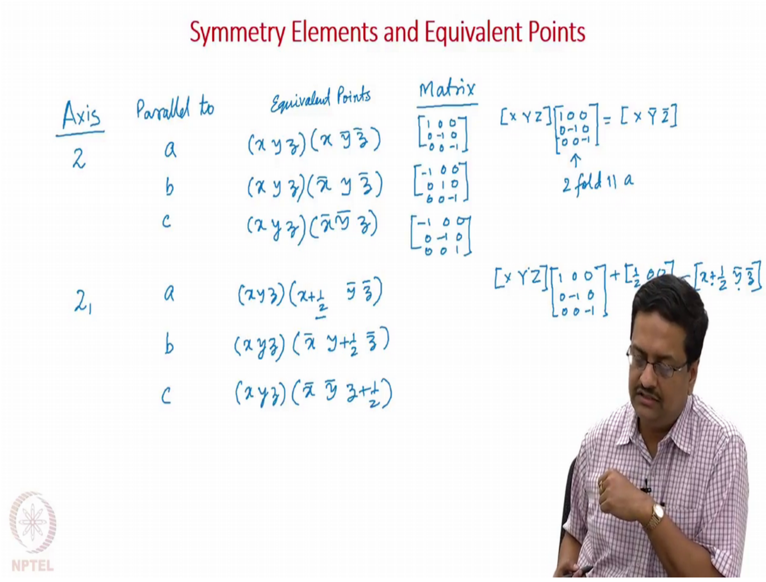

So, let us first identify the axis of symmetries. So, if we have a 2 fold axis these 2 fold axis can be parallel to a, b or c. So, it can be parallel to a, it can be parallel to b or it can be parallel to c. So, when we have such a situation the corresponding equivalent points will be different. So, for 2 fold parallel to a, the initial point is x y z the symmetry related point when the 2 fold is parallel to a; that means, the coordinate of x does not change, but y and z will have a negative sign in that. So, the corresponding new coordinate will be x, y bar, z bar remember anything minus we write in crystallography as bar.

So, similarly 2 fold parallel to b will have equivalent points x y z, and x bar, y and z bar. Similarly 2 fold parallel to c will have x y z, and corresponding x bar, y bar and z. This can also be done using a matrix method. The matrix for 2 fold parallel to a is this, which means if we start with a row matrix X Y Z and take a product of this with a 3 by 3 matrix corresponding to that particular symmetry operation in this case it is 2 fold parallel to a the result is X, Y bar Z bar. So, this matrix represents a 2 fold parallel to a. So, the corresponding matrix for 2 fold parallel to b will be minus 1 0 0, 0 1 0, 0 0 minus 1 and the same for c will be minus 1 0 0, 0 minus 1 0, 0 0 1.

So, the next set of symmetry elements are 2 1 screw which means it is not only rotation, but it has a translational component associated with it. So, this 2 1 can be parallel to again a b and c. So, now in this case what we have is x y z and this 2 1 when it is parallel to a the translation is along a and rotation is about a. So, when we rotated about a we ended up getting y bar and z bar as two coordinates keeping the x constant, but now there is a translation along x and how much is the translation the translation is half unit translation. So, it is x plus half. So, this becomes the new coordinate for 2 1 parallel to a. So, in the same manner x y z we applied to 1 screw parallel to b the new coordinate becomes x bar y plus half z bar and similarly x y z it becomes x bar y bar z plus half.

Note that this axis is parallel to one direction a, b or c. If it is parallel to a, the coordinate of a does not change sign coordinate of b and c that is y and z change sign on 2 fold rotation. And when we say that it is 2 1 screw the sign of y and z changes to minus and the translational component which is half is added to a when it is parallel to a. So, in matrix method the same X Y Z is then multiplied first by 2 fold which converts it into 2 and then you add a translational component half to the resultant value of this product what you end up getting is x plus half, y bar and z bar this is the matrix method of finding out the equivalent points for different symmetry elements.

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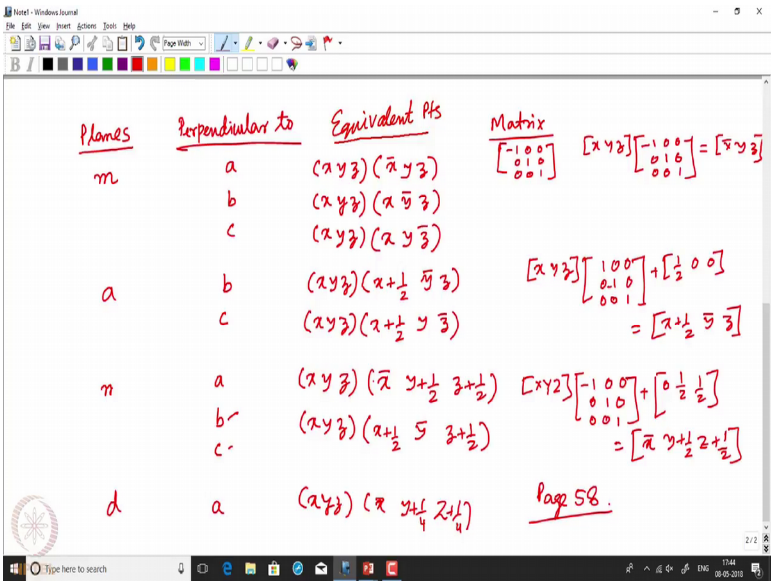

So, now in case of different planes, a plane can be perpendicular to axis the axis this group the principal axis or the screw axis is parallel to a, b or c, but when we talk about a mirror plane whether it is a mirror or a glide this mirror or a glide is perpendicular to a plane. So, these planes are designated in terms of perpendicular to and then we will write down the corresponding equivalent points.

So, now if I consider a mirror plane simple mirror m and it can be perpendicular to a, perpendicular to b or perpendicular to c. So, in that case the coordinates x y z when I say it is perpendicular to a the coordinate of x will change the sign, so x will become x bar and y and z will remain as it is. So, the equivalent points will be x bar, y z bar sorry; x bar, y z. Similarly x y z with mirror perpendicular to b will become x y bar z and x y z with mirror perpendicular to c will become x y z bar.

So, now we also need to learn: what is the matrix representation of a mirror. See, what is happening one coordinate is becoming negative, so the corresponding matrix will have only one term negative and others will not change. So, the operation is like this will end up giving you x bar y z. So, other than a simple mirror one can think of glide planes. So, I can have a glide and when I say a glide; that means, the translation is taking place along a and reflection is taking place perpendicular to either b or c.

So, when it is a glide perpendicular to b, I start with a point x y z it is a glide that means, translation is along a. So, a component of half will be added along a, and if it is perpendicular to b then b gets a negative sign and c remains as it is. Similarly if it is a glide perpendicular to c what should happen is x y z should become x plus half because it is a glide, so the translation is along a. It is reflection perpendicular to c that means, y does not change sign, but z changes sign. So, we write it as z bar.

So, the corresponding matrix notation will be a combination of a mirror operation and a translational component. So, the way we would write it is the following x y z minus 1 0 0, 0 1 0, 0 0 1 to that we add a component of half 0 0 to get x plus half, no, this minus is in the y because it is perpendicular there, so x plus half y bar and z. So, this is how one should write the matrix representation of a glide. So, I am not going to do b glide perpendicular to a or b glide perpendicular to c and c glide perpendicular to a or perpendicular to b, this I leave it to you to figure out yourself.

Now, I want to show: what is n glide; n glide is a glide in which the translation happens simultaneously in two directions; that means, the point moves along a phase. So, if I say n glide perpendicular to a, b or c we should have three different sets of coordinates. So, when I say n glide perpendicular to a; that means, x y z should immediately become x bar because it is perpendicular to a, but then the translation is along other two directions b and c. So, the coordinate of b and c should have a component of half added to it and it should become x bar y plus half and z z z plus half.

Similarly, n glide perpendicular to b should look like x y z it is perpendicular to b, so if b component is y bar and the half should be added to x and z. So, accordingly the matrix has to be modified in such a way that x y z, you multiply it by perpendicular to a means minus 1 0 0, 0 1 0, 0 0 1 to that we add 0 half half to get the final coordinate x bar y plus half z plus half.

So, in the same manner there will be d glide perpendicular to a. And in this case the translation is along the body diagonal and the translational component is only one-forth and then the coordinate is written as x bar y plus one-forth z plus one-forth. So, this is how the d glide gives you a new set of equivalent points. So, this is how one should be able to derive the equivalent points for different symmetry elements that we encounter in crystallographic symmetry these can be found in Staunton Jensen's book page number 58, 8 of this particular textbook which we have made as one of the main text books.

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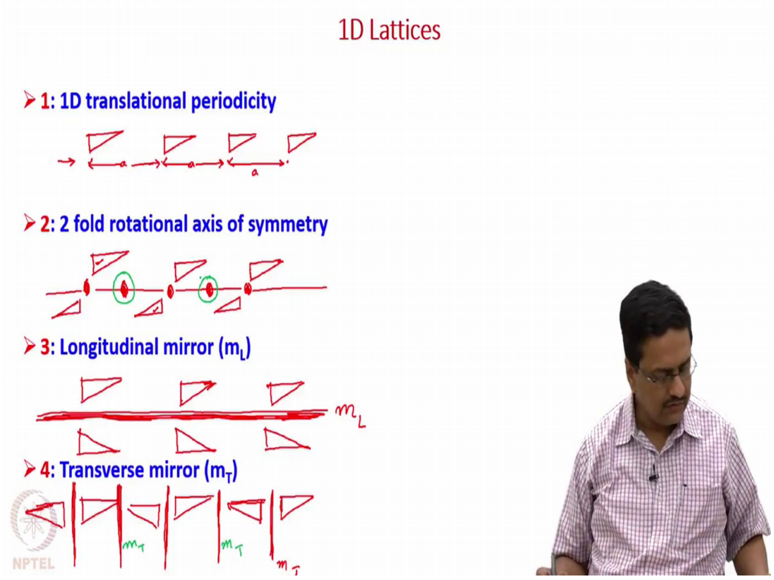

So, now we would like to go to build up when we talk about lattices we should first understand what is a 1D lattice, what are different symmetry elements that can be there in case of 1D lattice and how they those symmetry elements can be drawn and applied, and how that 1D lattice should look like. The 1D lattice, the first set of 1D lattice has only translational symmetry in it.

So, when we do that what we see is suppose I draw a triangle as my compound or molecule or motive and this triangle is translated in one direction at equal distance. And this is the diagram for 1D lattice which has only translational symmetry. The distance between the two lattice points is same. So, that is the edge length of the lattice. The second type of one dimensional lattice may contain a 2 fold symmetry. So, if I draw a same type of triangle and if I have a 2 fold symmetry present here, what will happen? This triangle will rotate and generate another triangle here. So, now this 2 fold axis makes the equivalent point here. So, if this is x y z, this is x y bar, z bar or whatever.

So, now, if I have a translational component associated with it which is the most important symmetry in three-dimensional crystal I should have these three triangles on the top. And then if I apply the 2 fold symmetry at every lattice point where the length is a, I end up getting these triangles once again. So, this is the direction of translation and the edge length is once again a in both the cases.

So, now what we end up seeing is that the relationship between the point here and the relationship between the triangle there is also a 2 fold. So, the presence of two 2 folds next to each other has given lives to another 2 fold in the middle. This new 2 fold is a result of two existing 2 fold rotational axis of symmetry. So, this is the second one dimensional lattice.

The third type of one dimensional lattice contains a longitudinal mirror; that means, the mirror is along the length of the translation. So, if I have again the same triangle and then I have a translational related triangle like this; as I have shown in the previous slide that the mirror that we construct in crystallographic symmetry is a bold line. So, this is my mirror. So, that mirror generates the reflection on the other side. So, this mirror is called as longitudinal mirror because this mirror is along the length of translational symmetry.

The next type of 1D lattice contains a transverse mirror which means the mirror is perpendicular to the direction of translation. So, if I just draw the set of molecule the set of triangles as I was drawing earlier, this just a translation related triangle and I am considering that there is a transverse mirror like that there is a transverse mirror here and so on. These are transverse mirrors. So, what happens is that this particular triangle gets reflected on the other side of the mirror.

So, now what we are see that there is a new mirror general transverse mirror generated in between the two transverse mirrors. So, these two new transverse mirrors are generated mirrors, just like the 2 fold that was generated earlier when you had two parallel 2 folds at the lattice distance.

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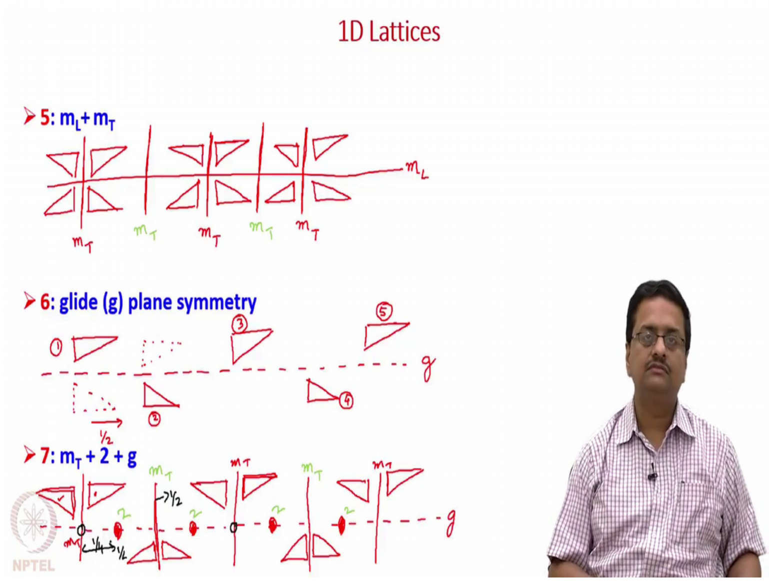

So, now we have the fifth type of lattice which is a combination of both longitudinal and transverse mirror. So, first I am going to draw the translation related components, then I will put the longitudinal mirror which then reflects the molecule like that and then I put the corresponding transverse mirror which is like this.

So, because of that mean this part this transverse mirror the molecule is reflected like that. So, now what has happened is there is a generation of new transverse mirror in between the lattice spacings. So, this is the longitudinal mirror, this is the original transverse mirror and the generated transverse mirrors are in between the two parallel transverse mirrors. So, this is the fifth type of one dimensional lattice.

As we have learnt about glide planes the glide planes are there in case of 1D symmetry as well. So, now, we will try to see how the glide planes translate the molecules in one-dimension. This is, these three are nothing but the translation related molecules and then I have a glide plane here as I indicated that glide plane is generally noted as dashed or dotted lines. So, I draw this glide plane like this.

So, now, if I had a simple mirror this particular triangle on top should have been reflected here, but this being a glide plane this triangle will have a translational component of half length along the direction of translation of the original object. So, this should move half way and come here. Similarly if you consider this molecule the corresponding mirror image should have been here, but they because of glide this moves to that. So, 1, 2, 3; 1 to 2 is a glide, 2 to 3 is another glide, but 1 to 3 is unit translation to the next unit cell and then three will have a glide related object somewhere here as 4 and the 5th object goes there which is again a glide relation between 4 and 5, but 3 to 5 is a translation relation.

So, now the last type of 1D lattice that we can construct contains all the three symmetry elements that we have learnt till now, transverse mirror, 2 fold and a glide plane. So, let us first draw the first object and the corresponding translation related objects which is the most important symmetry, and then we are drawing the corresponding transverse mirror. So, as a result of this transverse mirror we should generate the mirror image of the object, and then as we indicated there is a glide so that glide is along the direction of this translation. So, which I am drawing here because of that glide what happens is this, this object gets translated there, the object which is here gets reflected and translated there.

Similarly, these two are reflected and translated here and you generate another transverse mirror in between right and then on careful observation what we find is that there is a 2 fold which has been already generated we do not need to create anything special to show that there is a 2 fold. So, we have a glide, we have original transverse mirrors, then we have got the generated transverse mirrors, and then we have the generated 2 folds at one-fourth along the edge length. Because the edge length is from this point to that point, and the generated transverse mirror is at halfway, and this 2 fold is generated at one fourth from the origin.

So, this is how it looks for 1D lattice symmetry. There are 7 different 1D space lattices as I have drawn one by one, and in the next class we will start learning about 2D space lattices and their symmetries. And we will see how these symmetry elements, mirrors, glides and 2 folds generate a large variety of 2 fold lattices.