Solid State Chemistry
Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture – 16
Combining Symmetry Operations, Translational Symmetries

Now, we will start the 4th week of this course. In this week, I will continue the discussion on Symmetry Operations. And we will move to a different kind of symmetry, we called translational symmetry which is only seen in crystals. And so in this week I will be talking mostly about translational symmetry and I will also give some idea about why we learn about symmetry operations. And we will also talk about how you combine various symmetry operations.

So, in the first lecture of this week that is I will that is this lecture, I will talk about Combining Symmetry Operations and about Translational Symmetry. So, week 4, the 1st lecture we will be talking about combining symmetry operations and we will introduced the idea the general idea of translational symmetries.

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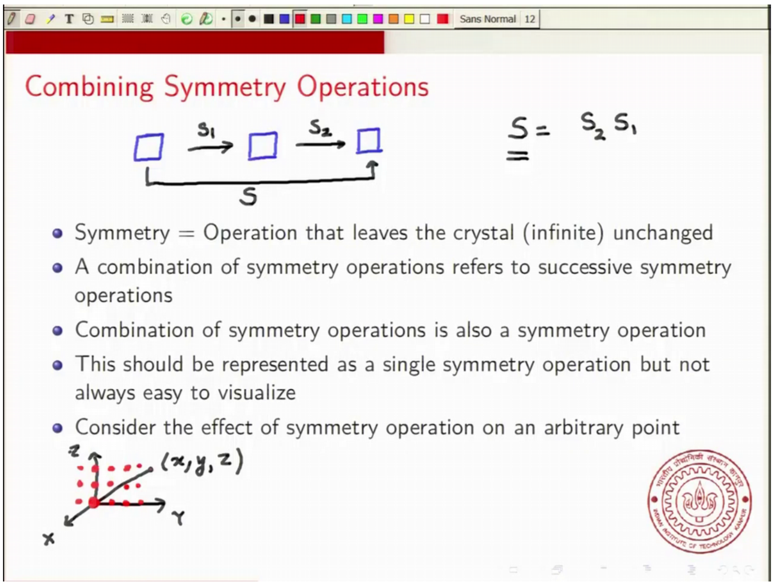

So, let us recall that a symmetry operation is an operation that leaves the crystal unchanged, and we should keep in mind that it is an infinite crystal. So, the crystal x tends to infinity in all directions ok. So, it is an operation that leaves that crystal unchanged ok. So, if you do a symmetry operation, you cannot distinguish the resulting crystal from the original crystal.

So, now it is very obviously clear that if you do one symmetry operation and then you follow it with another symmetry operation, then you will again leave this crystal unchanged. So, it is very obvious that a combination of symmetry operations will leave the crystal unchanged. So, a combination of symmetry operations is also a symmetry operation.

So, what we mean by a combination of symmetry operation is, you do symmetry operations successively. So, and we will see examples of this. Now, you can look at a combination of symmetry operations as some new symmetry operations. So, let me say that if you have a; if you have a crystal ok, let me show this in blue color ok. And you do a symmetry operation, let me call it S 1; S 1 is a symmetry operation ok.

Then you get a crystal that is identical ok. Of course, the I mean when you have transformed it, but essentially you cannot tell the difference between the original and the final configuration ok. Then you if you do another symmetry operation S 2, then again S 2 will leave the crystal unchanged. So, overall the crystal will be unchanged. Now, but you did these two symmetry operations, now you can ask the question, can I do a single symmetry operation that corresponds to both these symmetry operations ok, can I do a single symmetry operation ok.

Clearly to go from here to here, again you are leaving the crystal unchanged. So, it will be an it will be a single symmetry operation ok. And we express this relation as s equal to, so first you operate by S 1 first you act by S 1 then you act by S 2, so, it is shown in this order. So, typically we since the symmetry operation acts on the crystal, we can say that this symmetry operation on a crystal is equivalent to first acting by S 1 and then by S 2.

So, now sometimes you can easily see what this symmetry operation is, what this combination of symmetry operation is. Sometimes it is not easy to visualize what this combined symmetry operation is. And a general way to look at symmetry operations and to see how the product of symmetry operations acts is to consider the effect of a symmetry operation not on the entire crystal, but on one point in the whole crystal ok.

So, for example, we are thinking of something like this that if you have; if you have these coordinate axis x, y and z ok and you have some point somewhere in the crystal ok and this is a point in the crib this is a point in space ok and it is also a point inside the crystal. Now, how the crystal will have atoms everywhere, crystal will have its atoms whatever be the; whatever be the symmetry of the crystal.

So, these are the crystal atoms now and this is one point somewhere in the crystal ok. So, in the middle of all these crystal atoms, there is some point, some arbitrary point ok and we ask how this arbitrary point transforms on a symmetry operation.

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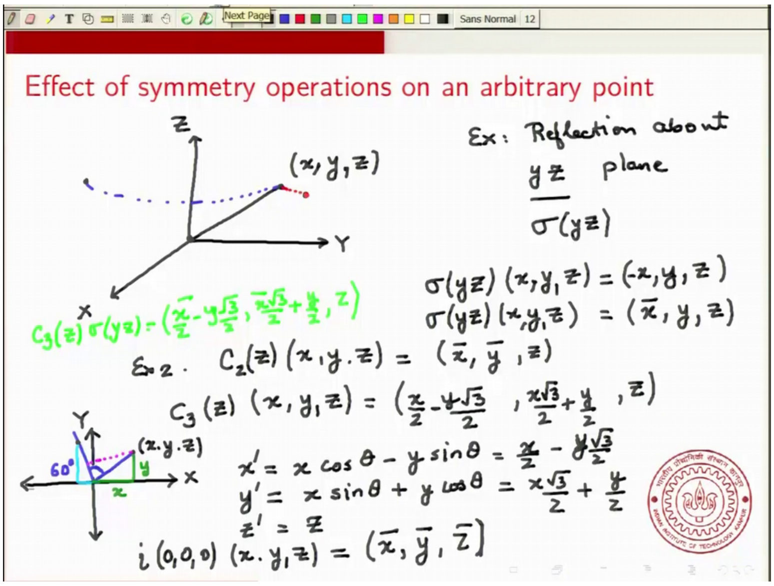

So, what we are doing again is to take some arbitrary point ok. The arbitrary point that we are considering will have coordinates x, y, z ok. Now, when we perform the symmetry operation on the crystal, then well also perform it on this arbitrary point ok. And at this point we will get will go somewhere. For example, suppose I do an example let us say you; let us say you have a symmetry operation of a reflection about let us say y z plane or y z plane.

So, if you reflect this point about the yz plane ok, then you can see that what will happen is that and let me use the symbol sigma, then let me denote this by sigma yz. So, if you, so what we want what we are saying is that if you take this operation, so this operation sigma yz, if you operate it on this symmetry point x, y, z ok; so, you take this point ok.

Now, you can see that when you reflect this point about the y z plane, then the you will get a new point. So, you are reflecting about the y z plane which is a plane of the screen. So, if you reflect it, then if this point is located above the screen of paper, it will go below the screen of paper ok. So, the new point will be behind the screen of paper ok, if the original point is above the screen of paper. And you can easily see that the new point since you reflected about the yz plane will have the same this new point will have the same y z coordinates, but its x coordinates will be changed to minus x. So, its x coordinate will change to minus x, but its y and z coordinates will remain unchanged ok.

Now, sometimes I mean especially in crystallography, we represent this minus sign as a x with a bar, y, z and we leave. So, the minus axis is represented as x with a bar. So, what you can say is that this sigma y z operated on x, y, z gives you this new point which is minus x, y, z ok. You can do this for other operations too. So, let us take an example let us rotate this point by 180 degrees about the let us rotate it about the z-axis.

In this case, you can see what will happen. So, if I take this point and rotate it about the z-axis ok, then this point its x and y coordinates will not change or rather its z coordinates will not change, but its x and y coordinates will change. So, if you rotate it by; if you rotate it by 180 degrees, C 2 corresponds to rotating by 180 degrees about the z-axis, then you can see that the new point will have the same z coordinates ok.

Now, what about the x and y coordinates. Now, you can again see that the x coordinate will change sign the y coordinate and the x coordinate will change sign, so you will get x bar y bar z ok. They will have the same value, but they will change sign. Now, these are fairly simple to see. So, things like C 2 and sigma etcetera are quite easy. Now, let us take something that is slightly more difficult. Let us take let us consider C 3 acting on the z x about the C 3 that is located along the z-axis acting on the point x, y, z ok.

Now, C 3 operation corresponds to rotation by rotation by 60 degrees ok. So, you are rotating by 180 by 3 that is 60 degrees. So, if you take a point x, y, z and rotate by 60 degrees about the z-axis ok, now we can see; we can see what will happen. So, first of all the z-coordinate will remain the same. So, we will just leave the z-coordinate as it is. Now, what about the x and y coordinates ok, now the x and y coordinates to know what will happen we will draw this picture slightly differently, we will show; we will show it in the x y plane ok. So, the z-axis is coming out of the plane of paper.

And let us consider a point is now the x and y coordinates of this point ok. So, we do not care about the z coordinate, because it is remaining unchanged. So, if there is a point with coordinates X Y Z then after rotation by 60 degrees you can see what happens. So, you will have this point and you rotate it by 60 degrees, you will get some point that is this. So, looks more like looks much larger than 60 if you take slightly smaller. So, you take something like this and you will get a new point that is located right here.

Now, the question is what is the relation between the coordinates of the original point and the coordinates of the new point. So, if this original coordinate had these coordinates so x and y, so this distance is y, this distance is x ok. Now, this angle is 60 degrees, this angle is 60 degrees. Now, this new point has some new coordinates. So, this is the new coordinates ok, the new x and y coordinates ok.

Now, if you want to it takes a little bit of work to work out the new coordinates ok, if you have to work out these new coordinates, you have to rotate by 90 degrees by 60 degrees and work out these coordinates. Now, this turns out to be a little bit more work, but not a whole lot ok. So, the new point we will have the following coordinates. So, you can work it out the following way.

So, so if you take this angle 60 degrees ok and you imagine that you drop or you can eventually work this out and you will get; you will get something like this, x by 2 plus y the root 3 minus y root 3 by 2. So, it is essentially x times cosine of 60 degrees minus y times sin of cos 60 degrees ok. The other term is the y coordinate is x root 3 by 2 plus y by 2, so that is x times sin of 60 degrees plus y times cosine of 60 degrees.

So, you can use; you can use the general relation x cos cosine of theta plus y minus y sin theta uses x prime this is for rotation by theta degrees about the z-axis. Y prime the new y is equal to x sin theta plus y cosine theta and the new z is equal to the old z ok. So, you can see now this since cosine theta is equal to cosine of 60 is half. So, you get x by 2 plus x plus y root 3 by 2 that is a new x coordinate. So, the new x coordinate is x, x by 2 minus y root 3 by 2, the new y coordinate is x root 3 by 2 plus y by 2 ok. And you can verify this very easily new z coordinate is nothing but the old z coordinate ok.

Now, this way you can work out all the symmetry operations. For example, if you invert about the origin ok, so if you do an inversion about the origin, so you are doing an inversion about the origin. So, you (Refer Time: 17:08) 0, 0, 0 as the point of inversion.

And if you invert this point x, y, z, you can easily see that it goes to minus x or write it in terms of in the notation that we have been using x bar, y bar, z bar ok; now, this is very useful.

So, this idea of symmetry operations on an arbitrary point is very useful, because now you can you can easily see the effect of combination of symmetry operations. So, you can do C 3 followed by sigma; so, we can easily do C 3 followed by a sigma ok. And what you will get is you will get you will suppose I do suppose I do let me write it here. So, suppose I do C 3 of z operated on I mean first sigma of y z ok, that means, first you do sigma y z then you do C 3.

So, sigma y z will give you x bar y z. Now, C 3, we will take x y z to this. So, all I do is I just replace this by x bar. So, I will get x bar by 2 plus y root 3 by 2 or minus y root 3 by 2, and then you get x bar root 3 by 2 plus y by 2 and you will get z ok.

So, the only difference is that only difference from the C 3 operation was that you replaced x by x bar and that is a consequence of this sigma y z. So, basically you can easily combine symmetry operations and you can find the effect of this combination of symmetry operations ok. Now, sometimes the combination of symmetry operations can easily be identified as another symmetry operations.

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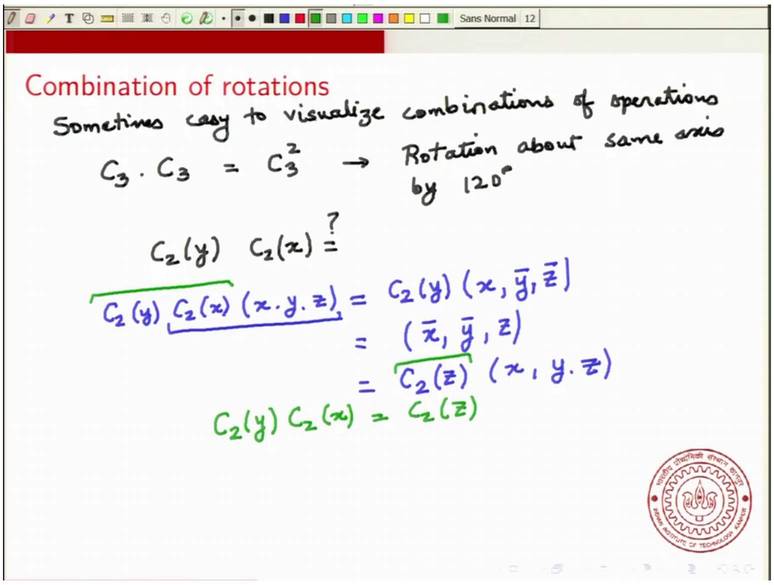

So, it should emphasize that this is only sometimes easy to visualize combination of operations ok. So, let us take some examples ok. And sometimes they are easy to visualize, sometimes they are not. Now, first thing is if you take rotations about the same axis ok, then you will get another rotation. So, for example, if you do; if you do; if you do a C 3 followed by a C 3 ok, two successive operations.

This will be denoted as C 3 square which is same as rotation about same axis. So, if C 3 corresponds to rotation about an axis by 60 ok, then C 3 square corresponds to rotation about the same axis by 120 degrees ok, by those C 3 square corresponds to rotation by 120 degrees.

Another example suppose I take C 2 x and I follow it by C 2 y suppose I take C 2 x times C 2 y ok. Now, what does this give? So, now, if I take C 2, so let us consider an arbitrary point. So, let us consider C 2 y times C 2 of x operated on an arbitrary point. So, if I take C 2 of x operate at an arbitrary point, then by the same thing we saw we just saw ok, this gives you so the C 2 y is as it is now I am just doing this part. So, this will give me x, it will keep the x coordinate same and it will change the y coordinate and the z coordinate ok. So, again the assumption the C 2 y is C 2 about the y-axis. So, C 2 x is C 2 above the x-axis and C 2 y is C 2 about the y-axis.

Now, if I do C 2 y on this point x, y bar, z, it will keep the y coordinate the same and it will change the signs of the x and z quadrant. So, you will get x bar y coordinate to be the same, it will change the sign of z bar of z bar. So, it will become back to z ok. And you immediately notice that here, here what I got is something that looks like a z, z, z coordinate is unchanged, but the x and y coordinate have flipped sign.

So, what you can see is that this is nothing but C 2 z time operator on the original point ok. So, what we have shown is that C 2 y times C 2 x operated on this point is the same as C 2 z operated on this point. So, we can write the relation between the symmetry operations. C 2 y, C 2 x is equal to C 2 z ok. This is a very special case where we could easily see the relation between the rotations. And I should emphasize that you cannot always see this ok. And in this particular case we see easily that the combination of these two rotations is another rotation ok.

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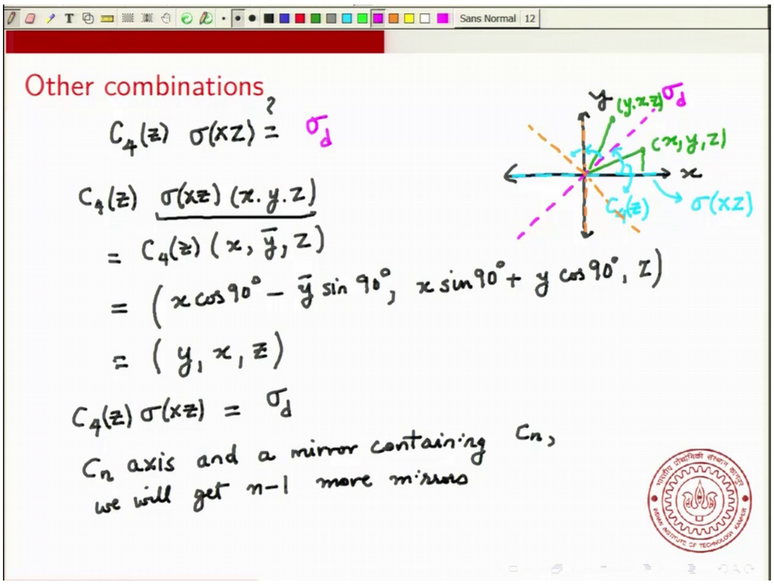

Let us look at some other combinations ok. Let me this is a again a very well known example in molecular group theory ok. Suppose I take; suppose I take sigma of x z. And I operate it operate on it by some let me choose C 4 and the C 4 is about the z-axis. So, first I am operating by sigma x z and then by C 4 ok. Now, let me show it pictorially ok. so, we are taking sigma about the x z. So, I will show it on the on the xy plane. See on the xy plane the z-axis is coming out of the plane of paper ok.

So, sigma xz is essentially perpendicular to this. So, it lies along let me show it in a different color. So, sigma xz is this that means, it is a mirror that is along the x-axis and it is coming perpendicular to the plane of the paper, so, this is your sigma xz. Now, what I am doing is I am doing a succession of two operations, I am operating by sigma xz first and then operating by C 4 ok.

Now, what do you get ok, now to do this. So, let us consider an arbitrary point. So, if you consider an arbitrary point x, y, z and you operate it by sigma x z and follow it by C 4. So, if I do this operation, what I will get is. So, I am just doing the second operations. So, I am just doing the second operation that is this operation which will be the first thing that will operate on this x, y, z point.

And what you can see it will keep the so sigma x z ok, we are reflecting about the xz plane. So, it will keep the x and z coordinates the same, it will just change the sign of the y coordinate. So, you will get x, y bar, z. Now, what does what happens when C 4 acts on this point ok. Now, to do this you need to know what is the effect of C 4 ok; C 4 is rotation by 90 degrees ok. So, C 4 will be rotation by 90 degrees.

Now, now cosine of 90 degrees is 0, and sine of 90 degrees is 1 ok. So, what it will give you is, so it will be x times cosine of 90 degrees minus y bar times, because the sin of 90 degrees that will be the new x coordinate. The new y coordinate will be x times sin of 90 degrees plus y times cosine of 90 degrees and the new z coordinate will just be the original z coordinate. So, these will be the coordinates. And if you just go ahead and work it out, we will get minus of y bar minus of y bar is nothing but y and sin 90 is 1.

Similarly, you have x sin 90 that is just x y cos 90; cos 90 is 0. So, you do not have to worry about that, so, you get something like this ok. So, you get something that keeps the z coordinate the same ok, but changes the x and y coordinate ok. So, this combination of operations ok, so this combination of operations keeps the z-coordinate the same, but swaps the x and y ok.

Now, the question is what would be something that does this ok. And the answer is the following thing would do it. So, if you reflect about a mirror that looks like this. So, now this corresponds to reflection about a mirror about this mirror. So, if you reflect an arbitrary point about this mirror, so I will just show it again. So, if you have an arbitrary point ok, if you reflect it about this mirror, then you can see that x and y coordinates will get swapped; so, the new point ok.

So, if this was your x, y and z, then this new point will have y, x, z ok. So, essentially what we identified is that C 4 z into sigma x z, this is equal to sigma and we will give this a name this is in molecular group theory this is given the name sigma d. So, we will just be consistent with that notation. So, it is a diagonal and it is actually, actually, this perpendicular to the z plane ok, we do not need to bother about that, but basically we are we can we can do a comment.

So, what we are seeing is that a rotation followed by a reflection gives you this rotation. Now, what is to be kept in mind is that the axis of rotation is a z-axis. So, the axis of rotation that we have considered as a z-axis and this lies in the mirror plane ok. Now, if you have; if you imagine doing C 4 z on sigma d ok, then what you will end up with is sigma y z ok. So, what you saw is that this C 4 operation in some sense, you can think of it the following way you can think that the sea for operation took this mirror this sigma x z mirror which is shown in blue and converted it to this sigma d mirror ok.

So, this is the operation, this is like a C 4 z operating on the mirror on the mirror itself ok. And you can only do this when the axis of rotation is in the plane of the mirror. So, and if you do this again, if you do; if you now operate C 4 on the this mirror, you will get a mirror along the along the y z ok. And you can you can continue and you can show all these you can generate more mirrors.

What is to be kept in mind is that while we did this ok. So, you can actually show that if you had a C n axis and a mirror containing C n ok, then we will get n minus 1 more mirrors ok. So, if you do by C 4, you will get this; if we do again by C 4, you will get another mirror that looks like this.

So, there are so basically these additional mirrors are generated using this C 4. So, if you just had a sigma x z, you operated by C 4, you will get sigma d and then you operate again by C 4, you will get this other mirror that is same as sigma y z. If you operate it again, you will get this other mirror which is another sigma d ok. So, you so from this one mirror you generated three, three other mirrors ok. So, same way if you have a C n axis and a mirror containing the C n we will get n minus one other mirrors.

Now, what is to be kept in mind is that these are very simple operations that we considered where, where we could actually identify, the identify; the identify the product easily. So, and we could also classify them in terms of we could have we could just by visually inspecting, we could we could see that this product turned out to be the sigma d I just by visual inspection of this of what we got. You cannot always do that sometimes the product of operations, it is not obvious what the combination of symmetry operations is. We will leave this here now I will just mention and I will just talk a little bit about translations as symmetry operations.

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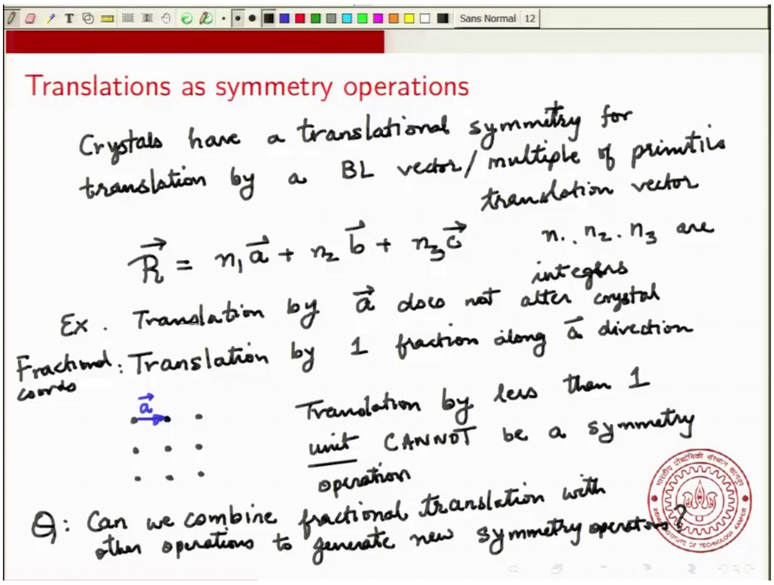

So, what I want to say is that so crystals have a translation symmetry ok. What is the translational symmetry of the crystal ok? So, if you take an arbitrary point ok, so if you take x, y, z or actually hatchery I should say it differently. So, if you translate translational symmetry for translation by Bravais lattice vector. So, if you translate it by this vector ok and which is the Bravais lattice vector or in some cases it can be the unit vector of the crystal by the primitive translation vector or multiple of primitive translation vector.

So, for example, if we consider just a lattice instead of a crystal, if you just consider a lattice ok and then you know that you translate any point by a vector R which is given by n 1 a plus n 2 b plus n 2 c ok. Then you will get; you will get where, where n 1, n 2, n 3 are integers, then you will get you will get essentially an identical point, you will get; you will get the same crystal there would not be any change.

So, now let us for simplicity let us take n 2 equal to n 3 equal to 0. So, if n 2 equal to n 3 equal to 0, so we will take the example. So, translate by a does not alter crystal ok. So, this is actually the definition of the crystal that a definition of the class crystal and these primitive translation vectors.

Now, suppose so in fractional coordinates; so, in fractional coordinate, so this is translation by one fraction ok. So, one fraction along a direction that means so instead of saying translation by a you say you translate by one along the a direction ok, it is and then and then this is in fractional coordinates.

So, let us take an example suppose you take a square lattice. You take a let us say a crystal form using a square lattice. Now, if you translate it by if you translate every point by a distance a by 1 unit along this direction ok. So, if you translate every point by this ok, you will get an identical crystal, it is very easy to see that. So, now this is this symmetry operation is actually used to define the crystal. So, the translation by 1 unit along one of the crystallographic directions is used to define the crystal.

So, what we are interested in is suppose we translate by less than 1 ok, translation by less than 1 unit. Now, this it cannot be a symmetry operation, because we said that a is the, a is in some sense the smallest translation vector that gives you this identical crystal. So, if you translate by a less than this, then you then you would not get a it would not be a symmetry operation.

So, the question when we are discussing translation as symmetry operations. So, we can ask the question can we combine fractional translation that is translation by less than a which is not a symmetry operation with other operations to generate new symmetry operations ok. So, this is a question the answer is yes and we will see in the next two class how this is done. So, we will see that this leads to two new symmetry operations called the glide planes and the screw axis ok.

But we will do that in the next class. So, with this I will conclude this lecture. And here I have talked about combining symmetry operations, we talked about the effect of a symmetry operation on an arbitrary point. And then I also told about I introduces I introduced how to think about lab about translation as a symmetry operation. So, I will conclude this lecture here.

Thank you.