Solid State Chemistry

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Lecture –19
Symmetry and Symmetry Notations

Now, I will start the 4th lecture of week 4 of this course. In this lecture I will try to; I will try to give an idea of why we are interested in symmetries. We looked at all the point symmetries, we looked at the translational symmetries and now we want to ask the question; why symmetries are interesting and why did we do this whole exercise in the first place ok? So, week 4 lecture 4 will be topic of Symmetry and Symmetry in Notations. So, I will also show in this notation, so, I will show how these symmetry notations are usually depicted in the planar notation.

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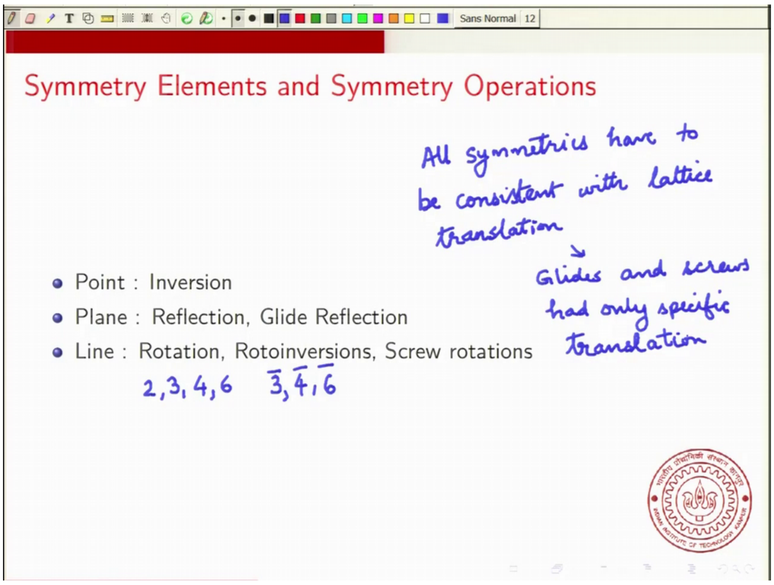

So, now we have seen the various symmetry operations the symmetry element. So, if you have a point, you can have an inversion, if you have a plane, you can have a reflection, you can also have a glide reflection whereas, if you have a line it can be a rotation axis, it can be an axis for roto inversions jetkor or it can be an axes for a screw rotation. So, these are the different symmetry elements and these are the various operations that are possible for each of the symmetry elements. Now notice that all these symmetry elements, all the symmetry elements that are listed have to be consistent with translational symmetry of the crystal.

So, all symmetries have to be consistent with lattice translation and by lattice translation I mean translation by one unit of the lattice one or more units of the lattice. So, all these symmetry elements have to be consistent with the lattice translation and this actually ensure that there are only few types of rotations and few types of reflections and so on ok, few types of screw rotations few types of rotoinversion. So, basically this ensured that you have only 2 3 4 and 6-fold rotations and similarly you just have I mean 2 bar is actually identical to inversion to i.

So, you just have rotoinversions of 3 bar, 4 bar, 5 bar 6 bar similarly you we saw that only certain allowed screw and screw rotations were present. Also one of the; one of the effects of this statement that all symmetries have to be consistent with lattice translation is that there were only very specific translations associated with the glides and the screws. So, glides and screws only had; so, the glides and screws had only specific translations, what I mean by this is that if when we were; when we were considering the glide reflections we always looked at either translation by half of the unit cell or quarter of the unit cell ok.

Now you can ask why did we not consider other glides by different amounts and it turns out that you do not need to consider them because an arbitrary translation by an arbitrary distance would not be consistent with the lattice translation. So, there are only certain kinds of translations that will be consistent with the overall lattice translation.

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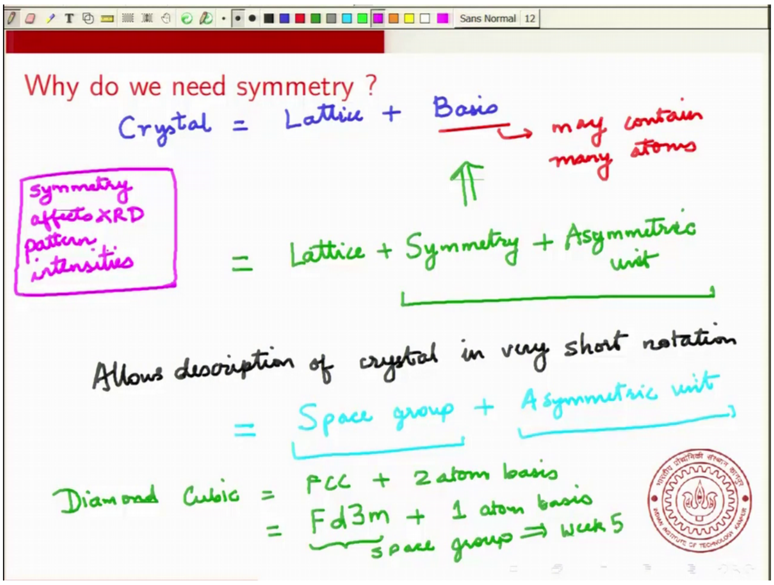

Now so, the question is why do we need symmetry? And I will give a few reasons why we need symmetry let us start with the following statement that we used. So, we had defined a crystal as a lattice plus a basis ok.

So, if what we mean by this is that if you want to generate the entire crystal you what you do is you take the basis atoms and you put them at each of the lattice points. You take the basis and put it at each of the lattice points and that will generate the crystal ok. Now the basis may be basis may contain many atoms and often it contains atoms of the same type for example, the diamond cubic structure can be thought of as an FCC lattice with a two atom basis and if you have a; if you have something like the unit cell of silicon then every atom is silicon.

So, the two atoms in the that form the bases are identical. So, now, what this suggests is that you could change this picture of crystal as lattice plus basis could be equivalently written in the following form. You could write it as a combination of lattice plus symmetry plus asymmetric unit or I will write specifically asymmetric unit ok. So, this corresponds to this is like a smaller version of the basis ok. So, you take the asymmetric part of the cell you apply the symmetries and then you do the lattice translations and you should get the entire crystal.

So, in other words this symmetry plus this asymmetric unit is what is generating the basis and what this allows us to do, this allows us to give to it greatly simplifies the notation for the crystal. So, allows us to describe crystal, description of crystal in very short notation. So, essentially you can use we will see this that we can describe the crystal using a very very short and brief notation you do need to describe what this our symmetric unit is ok. And we will see a specific example of this in the case of the we have already seen that if you take, we have seen it in the case of the diamond cubic ok.

So, now later on we will see that this lattice and symmetry they combine to form something called a space group. So, they are described by terminology called the space group so, we can really think of the crystal as a space group plus an asymmetric unit. So, this will be done in the following week ok. So, it is equal to space group symmetric unit ok.

So, really one advantage of symmetry is that you have a very very nice notation for these space groups and you have a notation for this and you have to actually say what the asymmetric unit is. So, if you specify this asymmetric unit that is the smallest repeating unit then you can really; you can really a specify the crystal structure.

So, you need the asymmetric unit and the space group. So, for example, we thought of this diamond lattice as. So, for example, we saw the diamond cubic as FCC plus two atom basis ok. And what we will see is that this is a space group I will not and the space group I will just write the name we will discuss this names a little later. So, F d 3 m this is the space group of diamond plus 1 atom ok. So, if you just; if you just say the one atom basis with this space group you will generate entirely you will generate the diamond cubic structure of something like a silicon crystal ok, we will discuss this later.

So, this is the name of the space group nomenclature. So, this is space group, so, this is this will be discussed in week 5 ok. So, this nomenclature will be discussed in detail in week 5 so, but, but essentially the idea is that you can describe this as this 1 atom basis which is the smallest asymmetric unit of the silicon plus the space group and you can do this for all sorts of groups, not just for silicon. So, for all crystals this can be done ok. There is another motivation for using symmetry and let me write it here and again we will just say that we will discuss this later.

So, symmetry effects I will just put it in a block here. So, this will be done again in some later week. So, symmetry affects X-ray diffraction pattern; pattern intensities ok. And we will see this we will see this later on when we are talking about X-ray diffraction ok. So, this will also be discussed later, but these are the reasons why we are interested in symmetry and why we spent such a long time discussing the symmetries.

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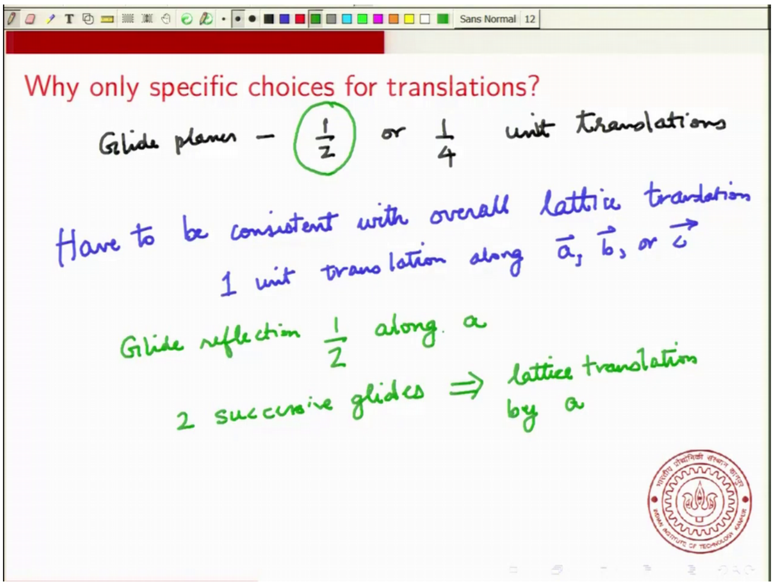

Next you can ask a question why this why there are only specific choices of translations ok. So, this is so, for example for glide planes we took only half or one-fourth. So, one-fourth was in the case of the diamond glide, but all other glides were characterized by half unit translations. So, the question is why only such fractions are allowed and we already said this ok, but the its about reemphasizing this it is.

So, the these are the only glides these have to be; have to be consistent with overall lattice translation ; that means if you translate by 1 unit along a along any of the axis a b or c should give you an identical structure ok, should give you a completely identical structure.

So, whatever glide planes you have should be such that if you they should be consistent with this overall lattice translation. So, for example, if you say a glide plane of half if you look at the half glide plane ok. So, you do a glide reflection of 1 by 2 and if you do this two times ok. So, if you do a glide reflection of 1 by 2 and let me take along a for example ok. So, 2 successive glides will generate lattice translation by a ok.

So, remember that glide reflection corresponds to reflection in a mirror and a translation along some direction in this take in this case we took the example of an a direction. So, now and its translation by half unit; so, when you do; when you do two successive glides ok. So, then the then you will end up reflecting again so, the second time you do it you will again reflect. So, you will come back to the original sense with respect to the plane of reflection and then you translate by a you will get shifted by a.

So, the effect of two successive glides is just a lattice translation by a in other words the two mirrors the two mirror reflections will cancel each other and what you will be left with is just by a translation by half a followed by another translation by half a, so, that is an overall translation by a ok. So, clearly this glide reflection is consistent with the symmetry of this overall lattice translation and similarly you can show even for the diamond glides ok, we can show that they are consistent with the overall lattice translations ok. And you can similarly show that there will be other glides that are not consistent with this overall lattice translation ok.

So, if you take; if you take arbitrary if you translate by some arbitrary distance then it could be that it is not consistent with the overall lattice translation ok. So, these are these are some of the reasons I mean these are not very easy to see to exactly work out, but at least you can see why you only use specific choices for these translations.

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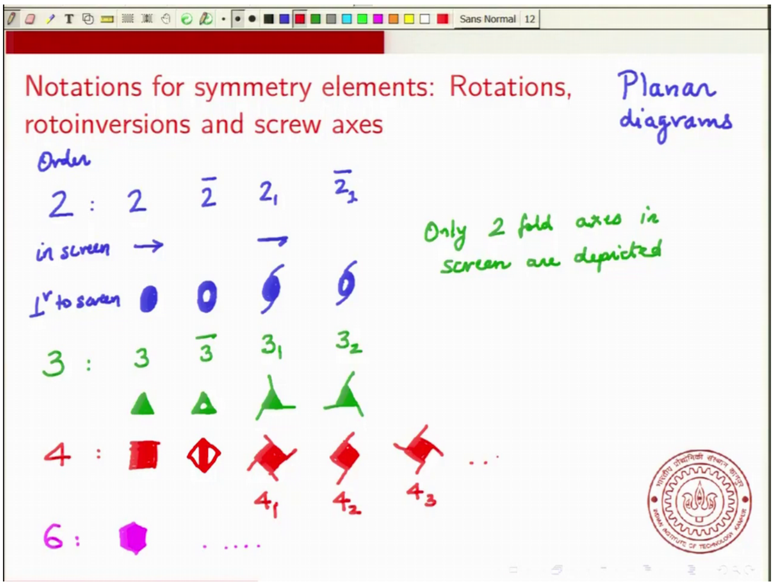

Now, let us look at the notations for different symmetry elements and we will these are usually shown on the on the planar diagrams. So, on the Planar diagrams you use these notations for symmetry representations and it turns out that using these notations we can actually generate the using these symmetry elements and any a symmetric unit you can generate the entire crystal ok. So, I am going to; I am going to talk about the different rotations for the rotations, roto innovations and screw axes. So, each of these correspond to some axes. So, you could have an axes and that could be a either an axes of pure rotation or a rotoinversion or a screw axes ok.

So, let us look at this notation. Now let us say you have a order to access or 2-fold axes ok. So, if you have a 2-fold axes now it could be a; it could be a pure rotation like a two axes ok, then the notation that is used is you. Now you could have a 2 rotation either in page in the screen in play, in screen that is in the screen or perpendicular to screen ok. Now if it is in the screen a 2-fold axes of rotation that is in the screen is shown by this arrow, a line with an arrow ok. So, that represents our 2-fold axes of rotation that is in the page a 2-fold axes that is perpendicular to the page is shown let me use a different ok.

So, that is perpendicular to the screen ok, is shown by an oval that is filled ok. So, an oval that is filled is used to show that there is a 2-fold axes that is perpendicular to the screen. Now they can be other 2-fold axes ok, you can have a 2 bar which is a 2-fold rotation plus an inversion and this is shown it is very similar to let us I will show a 2 bar that is perpendicular to the screen ok. So, if you have a 2 bar that is a 2-fold axes plus an inversion then you show it using this symbol.

So, it is a like this oval, but there is a small hole in inside to show that there is an inversion now there are other 2-fold axes that you could have. So, for example, you could have a screw axes, so, if you have a 2 sub 1 now. So, this corresponds to rotation by 180 degrees and translation by half the unit cell and this will show it; will show it by. So, if it is in the screen of paper will show it by this harpoon ok. So, it is half an arrow ok, so, a line with half an arrow line indicates that the rotation is in the screen.

So, its along this line and the harpoon indicates that it is a screw rotation, if it is perpendicular to the screen then you show a regular 2-fold axes, but you show it with this. And if you have a 2 bar sub 1; if you have a 2 bar sub 1 then you show it you show it like a 2 bar with this screw ok. So, this is a 2 bar sub 1 and we generally do not show the 2 bar axes in the screen of the paper in the screen. What else you can have for the screw axes you could have, I mean these are the these are all the possibilities that you can have for a 3-fold axes. Now let us go to a 3-fold axes and I will use a different color ok.

So, if you have a 3-fold axes ok, now there are many more possibilities in this case if you have a just a regular 3-fold axes you could have a regular 3-fold axes and usually you do not show any 3-fold axes that is in the screen only 2-fold axes in screen is shown ok. So, let me emphasize this point. So, usually only 2-fold axes in screen are depicted. So, in the screen only 2-fold axes is depicted, the 3-fold axes perpendicular to the page all the axes are did are depicted.

So , if you have a 3 perpendicular to the screen then you show it by a triangle or fill triangle, if you have a 3 bar then you show it by a triangle with a circular hole ok. If you have a 3 sub 1 then you show it by a fill triangle with these extensions here. If you have a; if you have a 3 sub 2 ok, 3 sub 2 is like rotation by minus 60 degrees and translation by one-third or you can say rotation by 60 degrees and translation by two-third and this will have this will show it ok. So, its just that the that the lines are in the opposite sense; what else can you have? You could have; you could have.

So, these are all the possibilities that you could have here, now I will just briefly show the other axes I would not show all the possibilities. So, for 4-fold axes it is shown by a triangle that is a 4 fold, a 4 bar will be shown by a triangle with a circular hole and in this case the 4 bar is actually shown in this direction like a diamond. And again all these axes are perpendicular to the screen and I will just; I will just show 4 sub 1. So, a 4 sub 1 would look like this; well actually 4 sub 1 is again shown like a square that is it and 4 sub 1 is shown this way now you could also have a 4 sub 2 you could have a 4 sub 2 and I will show it.

So, the 4 sub 2 is shown by now only two lines are drawn. So, this is 4 sub 2, so, 4 sub 1, 4 sub 2 and if you want to show 4 sub 3 you show it again we use the fact that its like a 4 sub 1, but the lines are drawn in the opposite direction in the perpendicular directions ok. And similarly if you have a; if you have a 4 sub 3 with an inversion then there will be; there will be there be an empty circle in the middle ok; now I will just briefly mention the other two. So, if you have a 5 if you have a 6-fold axes.

So, I will just mention very briefly what how you show 6-fold axes. So, 6-fold axes is shown by a hexagon a filled hexagon and you can use very similar depictions for all the remaining; all the remaining axes. So, all the remaining 6-fold axes will be shown in a very similar manner and so, on similarly you have more of these 4-fold axes ok.

I just wanted to show some of these you might see them, you might see structures that are typically this way ok. I am not showing all of them just showing a few of them; so, that you get a general idea of what how rotation axes are represented in the planar figures ok.

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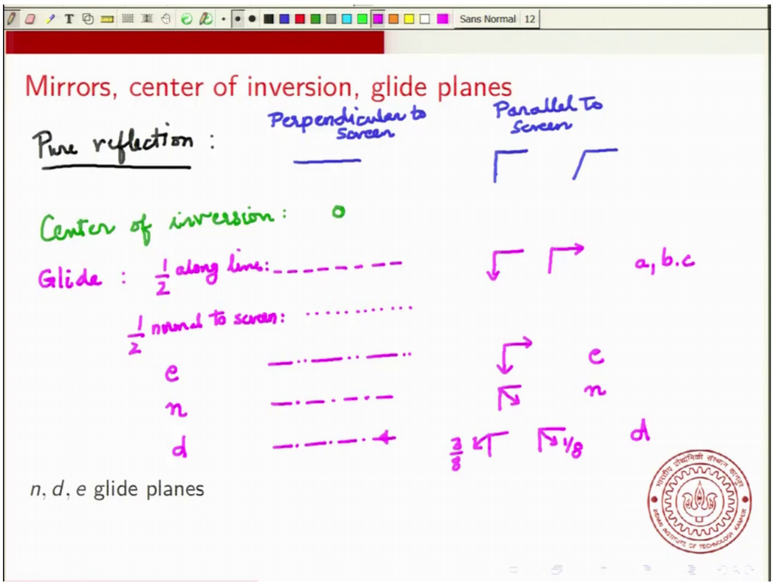

What about mirrors. So, mirrors mirror is a plane of reflection and if it is a pure reflection and let us say; let us say that if it is perpendicular to the plane of the paper it is in the plane of this if it is perpendicular to the plane of the screen or in the screen in the plane of the screen. So, those are the two possibilities ok. So, in so, I will say; I will say perpendicular there are to screen in other places parallel to screen. Now, if it is a pure reflection that is perpendicular to the screen then it is shown by a solid line, a solid line is a symbol for a pure for a mirror that is perpendicular to the screen if it is parallel to the screen then usually you draw lines along the crystallographic axes along the.

So, this indicates a reflection that is parallel to the screen. Now in case your cell is not is not its tetragonal cell or then you will have something like this in case the angle is not 90 degrees the angle between a and b is not 90 degrees then you will show it in this way ok. Then what else can you have? You can have a center of inversion, look will you can have a center of inversion and that is a unique.

So, center of inversion and that is just denoted by a circle where empty circle then finally, you could have glide planes and you could have a variety of glide planes ok; now I am not going to. So, these are glide planes or mirror or mirrors ok. So, and they there are a variety of notations for glide planes depending on depending on what kind of glide plane it is and what is the direction of the glide, what is the where is the plane located. So, in the first case when the plane is perpendicular to the screen then there are a few different notation. So, you could have now there are various symbols if you so you could have a dashed line and this indicates that the glide is, that the translation is half along line ok.

So, the translation direction is along this line ok; along this line that is shown the mirror is perpendicular to the screen translation is along this line ok. Now you could also have a translation of half, you could also have a glide plane that is perpendicular to the screen, but the direction of the glide is half, but normal to the plane normal to screen, in this case you use a dotted symbol. So, the direction of translation in the first case was along this line in this case it is normal to the screen, then if you have a double glide plane ok.

So, we talked about the e glide double glide I will not I will not discuss this in detail, but you can have; you can have something like this. So, this represents a double glide plane that is perpendicular to the screen. You could have a n glide ok; now the n glide is again if it is perpendicular screen its a line with a dot. So, it is a dashed dot line is an n that is a diagonal glide.

Then you could have a diamond glide that is d that is a diamond glide plane and this looks actually you mean you mean the symbol is very similar to the diagonal glide ok, but there is an arrow that is drawn there is an arrow to indicate that its a diamond glide plane.

So these are the various glide planes that you could have that are perpendicular to the screen when they are perpendicular to a screen. Now, when they are parallel to the screen we saw that the pure reflection is shown by this little angle similarly all the glides when the glide plane is parallel to the screen then usually since a. So, you could have; you could have several different glide planes for example, you could have a glide plane and if the direction of translation is along this axes ok, it could be a or c ok or you could have a glide plane where the direction is along some other axes that is shown ok.

So, the arrow shows the direction of the translation this could be a b or c then you could have a double glide plane; double glide plane which is which would look like this and e glide would have two arrows ok, that is an e when it is parallel to the screen ok. You could have a diagonal glide that is that would look like along some diagonal glide. So, that is an n glide and you could have a diamond glide which there are different notations you could have something like this is a diamond glide I am not going to go into this in too much detail.

Because we will not be using it too much during this course you could have things like this where the arrow shows the direction of the translation and usually this arrows since the length of this arrow will be denoted. So, if you have a one-eighth translation or a three-eighth translation in this case ok. So, that this will be the length of the arrows; now again this would be a diagonal this would be a diamond glide when you show it in the plane this is what it will look like ok.

So these are the general ways in which all the symmetry elements are represented in various planar representation.

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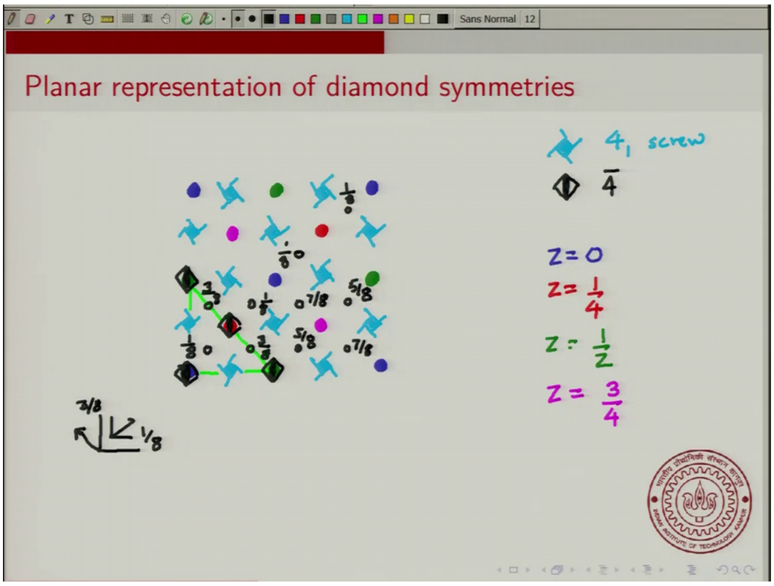

Now, now we will talk about the planar representation of diamond symmetries ok and here I want to show what the various screw axes look like. So, now, if you recall the planar representation of diamond it looked like this. So, you had the atoms at Z is equal to 0 this was a Z equal to 0 layer then you had at Z equal to one-fourth, you had these two atoms at Z equal to 1 by 4. Then you had at Z equal to half you had atoms at the edge centers and at Z equal to 3 by 4 you had you had points that were located here along this other body diagonal ok.

So, these are at 4 different values of Z and this was the representation of the diamond structure. Now let us look at the symmetries. Now you should keep in mind that we had, there is an inversion center right between these two ok. So, it is at its along there is an inversion center at Z equal to 1 by 8 ok; at 1 by 8. So, this inversion center is at Z equal to 1 by 8 and it is on the line that is bisecting these two points biasing this blue point and this red point ok. Now it takes a little bit more effort to see the other symmetries ok. Now I will show; I will show location of a 4-fold screw axes let me use this color.

So, there is a 4-fold screw axes that is located right here. So, there is a 4-fold screw axes that is located and on right at this point, you can verify this if you rotate by 90 degrees and then this red point will go directly below the green point and then you translate it up by, you translate it by one-fourth then you will get you will get this point. So, this is a 4 1 screw axes; 4 1 screw axes that is located there.

And now you can show that there would be another screw axes is symmetrically located at this point, but this would be a 4 3 screw axes ok, in the sense if you if you rotate it clockwise then this red point will be on top of the blue point and then you were to translate it down by one-fourth ok, alternatively you can translate it by a by three-fourth ok.

So, this is a 4 3 screw axes ok and similarly you can easily show that there will be a screw axes located here that will be that will be a 4 1 screw axes and there would be a 4 3 screw axes here. So, you can easily infer the presence of these screw axes and now additionally there is there is of course, the diamond glide plane ok. So, the diamond glide plane which is shown in the following way ok; so, the diamond glide. So, this is a diamond, this is a representation of the diamond glide that is 3 by 8 and 1 by 8 ok. So, so, you can easily show that there is a glide plane.

So, this that is parallel to the screen and it is a diamond glide plane ok. Now I do not I mean you can also show symmetry elements on the other parts of the diamond, you can I mean just as this same symmetry element would also be here ok. Similarly this symmetry element will be here and so on, you can just complete the whole. So, now you can also see that the asymmetric unit of diamond. So, the asymmetric unit of diamond is just this is the your symmetric unit ok. So, this small one-eighth corner is the asymmetric unit and you can essentially whatever is there here is seen in all the others.

So, for example, you would have a; you would have an inversion center between this red point and this blue point this will be located at three-eighth or sorry this will also be located at one-eighth, you would also have inversion centers here at one-eight and here at one-eight and there will be other inversion centers between other connecting points that will be located at different distances. For example, here you would have an inversion center located at. So, at no not here it will actually be located between this is at three-fourth so that is ok.

So, there will be an inversion center right here at 7 8 similarly there will be an inversion center here at 7 8 ok, there will be inversion centers located here and here and similarly there will be inversion centers located here and here ok. These will be at a distance of 3 8 and these will be located at distance of 5 8 and I am not showing in the other parts of this of this unit cell ok. Essentially, what I am trying to say is that you just need to know the symmetries of this asymmetric unit or what are the cement where are the symmetry elements and essentially you are done ok, now there are several other axes for example, now this is a 4-fold roto inversion axes.

So, there are 4-fold rotoinversion axes located right here. So, this atom has a 4-fold rotoinversion axes that is shown by; so, 4-fold rotoinversion axes is shown this way. Similarly there will be a 4-fold rotoinversion axes at this point and at this point ok. So, these are and similarly you can show that it will be at all these other points, but I am not showing them I am not bothering to show the remaining points. In fact you can show that there will also be a 4-fold rotoinversion axes right here ok.

So, there are several for each of these; each of these points each of the points in the in the diamond cubic lattice act as a 4-fold rotoinversion axes. So, 4 bar; so, there are also screw axes I am not showing them here ok, but there are there are also other screw axes and diamond which we had already seen earlier, we had we had seen some of the screw axes and diamond I will not; I will not show them in this figure because already we have shown lot of symmetries already in this. So, with this I will conclude this fourth lecture of week 4 of this course, in the next lecture we will summarize what we learnt in week 4 and then do some practice problems.

Thank you.