Solid State Chemistry
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Lecture – 20
Summary of Week 4, Practice Problems

Now, we will go to the 5th and final lecture of week 4 of this course, in this lecture I will summarize what we learnt in week 4 and then do one practice problem. So, week 4 lecture 5 we will have a Summary of Week 4 and Practice Problems ok.

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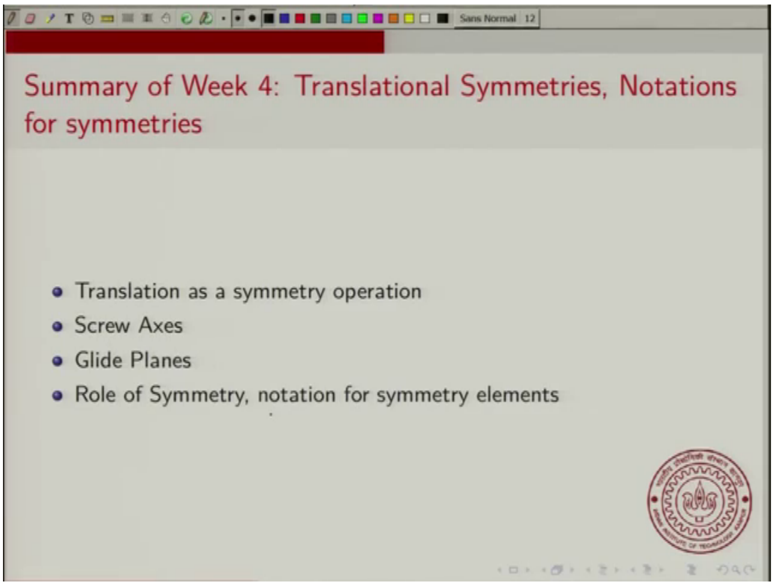

So, what did we learn in week 4 we learnt about translational symmetries and then we learnt about notations for symmetry. So, first we looked at how to view translation as a symmetry operation ok, especially with respect to lattice translations ok. Then we learnt about screw axes we learnt about glide planes and then finally, I talked about the role of symmetry as to why we need symmetry and then we learnt we saw some notations for symmetry elements ok. Now, so all this actually concludes the 2 week discussion on symmetries ok.

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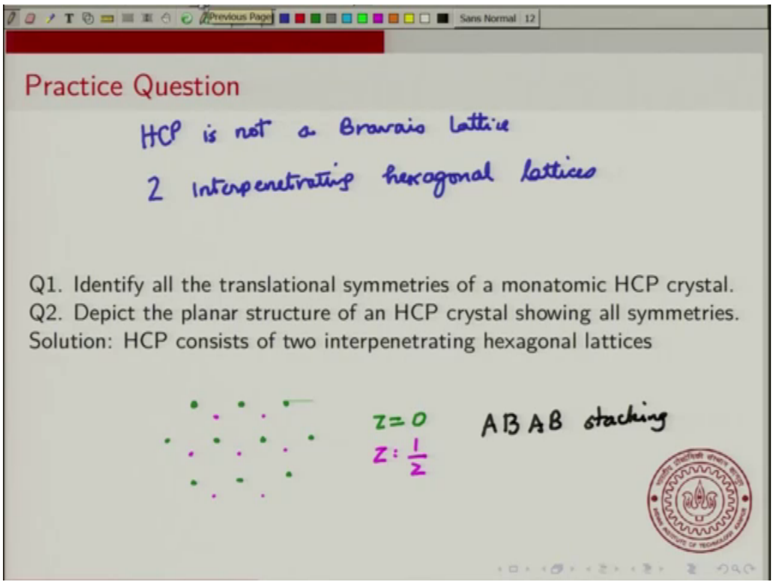

Now, let us look at one example here you are asked to identify all the translational symmetries of a monatomic HCP crystal and then you are asked to depict the planar structure of an HCP structure showing a HCP crystal showing all symmetries. So you should keep in mind that HCP is not a Bravis lattice, so HCP is not Bravis lattice and it consists of 2 interpenetrating hexagonal lattices ok. So, what does HCP look like I will just show you here. So, if you have let us say in the plane of the paper you can have one hexagonal lattice ok, that will be in this manner ok. So, this would be this would be a hexagonal lattice ok.

And this you can imagine this you can say it is at z equal to 0 and the it will be at z equal to 0 and at z equal to 1 and so on. The other hexagonal lattice which will be at z equal to half will be will be located this way so this is at z equal to half. So, it keeps alternating this way and it forms a it forms an AB AB type stacking. So, later on we learn about stacking of crystals and this corresponds to a AB AB stacking.

That means the z equal to 0 layer is followed by as the z equal to half layer and then the third layer is on top of z equal to 0. So, the atoms are stacked in all in layers of this form AB AB ok. Now, how do we show the and what are the translational symmetries of this HCP crystal ok.

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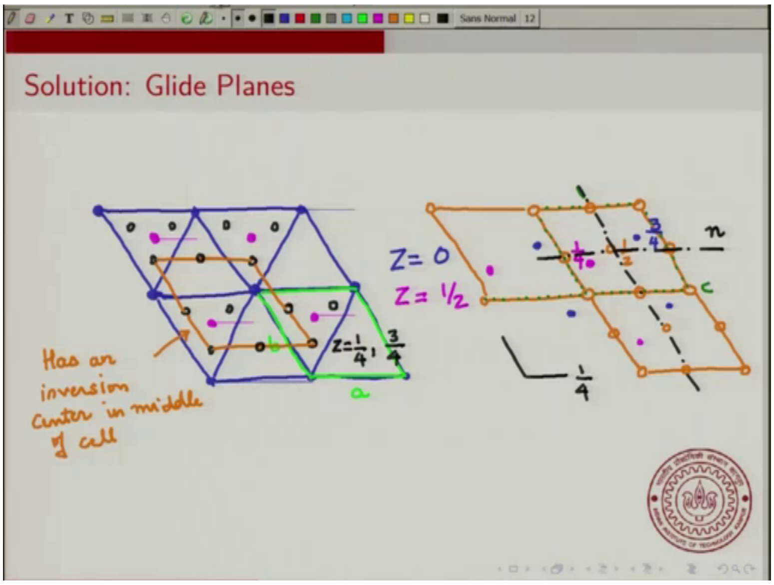

Now, let us look at the glide planes ok, now let us again show the now before we look at the glide planes its instructive to think what would be a suitable unit cell for this HCP; HCP lattice ok. Now, typically the unit cell is chosen in this manner, so you choose a cell of this way ok.

So, you choose a and b and c is perpendicular to the screen ok, so that is a typical choice of unit cell and now let me show that unit cell here . So, this is at z equal to 0 and then you have at z equal to half you have a 1 atom that is located right here. So, essentially there are 2 atoms in this unit cell ok, so if you look at this whole cell it will you see atoms in the corners and the net contribution of all those atoms is just 1 atom and then you see one inside the cell.

Now if you take the HCP cell and let me expand it a little bit just to illustrate the point ok. Now what you can see a when you expand it is the following that each of these; each of these; each of the planes has a 6 fold symmetry. So, each of the; each of the individual planes by themselves they have this 6 fold translate 6 fold rotation axis ok. So, if I just connect these just for ease of visualization ok.

So, now if you take; if you take this z equal to 0 plane it is a hexagonal lattice, so it has a 6 fold axis of rotation. However, since it is interpenetrating with this z equal to half there is not so that does not act as a 6 fold axis of rotation for the HCP lattice ok. The other thing that is slightly let me now show the unit cell that we wanted to consider. So, we wanted to consider 1 unit of this as a unit cell ok, this is the unit cell where a b and c is defined perpendicular to the screen ok. Now one of the things that is not obvious with this unit cell is the inversion symmetry of the HCP lattice ok.

Now, actually HCP lattice has an inversion symmetry and that inversion is with respect to a point that is right here, that is halfway between this corner point and this point inside the cell. So, this is a point of inversion and now sometimes its convenient to show the symmetries using this inversion point ok. Now this inversion point is located at z equal to 1 by 4 and end at the appropriate coordinates of a and b ok, but its located at z equal to 1 by 4 ok.

Now, to show the symmetries of now often what is done is to take is to show the symmetries with respect to this to this inversion point ok. Taking we want to illust we want to have a cell which actually captures this inversion center and there are several ways to do that I should also mention that there will be other inversion center. So for example, there would be one here all these are at z equal to 1 4 th and there will be similarly there will be one at z equal to z equal to 3 by 4 there would be inversion centers here .

So, sometimes we choose unit cells so that they capture this inversion this center of inversion is naturally captured and so for example, you might choose a unit cell that is in this formula like we use. So, if you choose this for example, as a unit cell where it starts from z equal to 1 by 4 and goes one unit up ok. Now you can see that all these are inversion centers ok.

So, all these become inversion centers and this is often now this cell this unit cell has inversion symmetry because there is a point of inversion right in the middle of this cell. So, just as z equal to 1 by 4 there is also a similar; there is also a similar point directly above it at z equal to 3 by 4 ok, there also be a point directly about above it at z equal to 3 by 4.

So, that the point at z equal to 3 by 4 will be at the center of this cell. So, a cell that is taken with these points has an inversion center in middle of cell ok. So, right in the center of this point so this point will be a point of inversion ok. So, let me draw this cell here so what it will look like ok. So, we will have points and you have so this is at z equal to 0 and half and 1 ok.

So, this is z equal to 0 and you have a point of inversion at z equal to half well ok, so I will just write this as half. So, these points are at z equal to 0 these are inversion points, now the question is in this the atoms are not located at the corners ok, say the atoms are located; atoms are located somewhere here and the other atom is and with respect to this cell this atom this.

So, this was located at half in the original cell in this cell a since its translated by it is already raised by one fourth this atom will be located at 1 by 4 and this atom will be located at 3 by 4. So, maybe I will use a different color I will use the blue color this is at 3 by 4. So, this is the same unit cell now it has 2 atoms, 2 points that are inside the corners there are no points at the corners and this is what we will use to; we will use to show the symmetries ok.

Let me show the other inversion centers there are also inversion centers here and here and here, here, here ok. So, I should mention that there will also be an inversion center right here and right here and this ok. So, these are the inversion centers in this unit cell and you can already see how you can already see that also you can easily see that the point at the center is a point at the flow inversion because if you invert about this.

This lattice point at one by this purple lattice point we will go to the blue lattice point and vice versa ok. Now we can show the other symmetry operations ok, so since you have this inversion you will have a; you will have in addition to this now we will first show that light planes ok. Now there is a glide plane that is so if you take a glide plane that is let me extend this cell then the glide plane will become clear. So, we will extend it here and this point will come right here and you will have this point that is right here ok.

Now the first thing that you will see is that if you look at a plane passing through this 1 by 4 passing through z equal to 1 by 4 ok. So, if you look at; if we look at a plane in the if you in the plane of paper passing through z equal to 1 by 4 this is a plane of reflection. So, its parallel to the; parallel to the screen, but at a height of z equal to 1 by 4 ok, so, that is a plane of reflection and that is fairly easy to see ok.

The next thing that you will see is that there is a glide plane that contains the a and c axis and this will reflect the. So now, there will be several glide planes in this crystal and in this lattice and let me show some of them. So, there will be a glide plane here and this in this so if you are reflect about this plane and you can translate; you can translate will be seen more clearly if I extend this cell.

So, let me extend it in this direction. So, you can see that if you reflect this point and translate along this line ok, if you reflect about this plane and well ok. So, if you reflect about this and translate along this line you will get you will end up at this point ok.

Similarly, if I so there is a glide plane in this direction there is a similarly there will also be a glide plane this way a glide reflection. So, you can see that if you reflect this point will come directly here and then you can do a translation to get to this point.

So, if you reflect about this you will end up here and then you translate it along this line you will get to this point ok. So, this these are some of the glide planes now what are the other now again just by symmetry of this unit you will have glide planes also here ok. There are several other glide planes in this HCP lattice I will show some of these ok. There is a diagonal glide plane; there is a diagonal glide plane that is located here and the symbol for a diagonal glide plane is a line and a dash ok, so this is a diagonal glide.

So, n glide plane, this is a c glide plane and so on you can show several other glide planes that are symmetrically reflected in this. So, if there is one here they will also be one in this direction ok, so these are the glide planes in this diamond cubic lattice ok.

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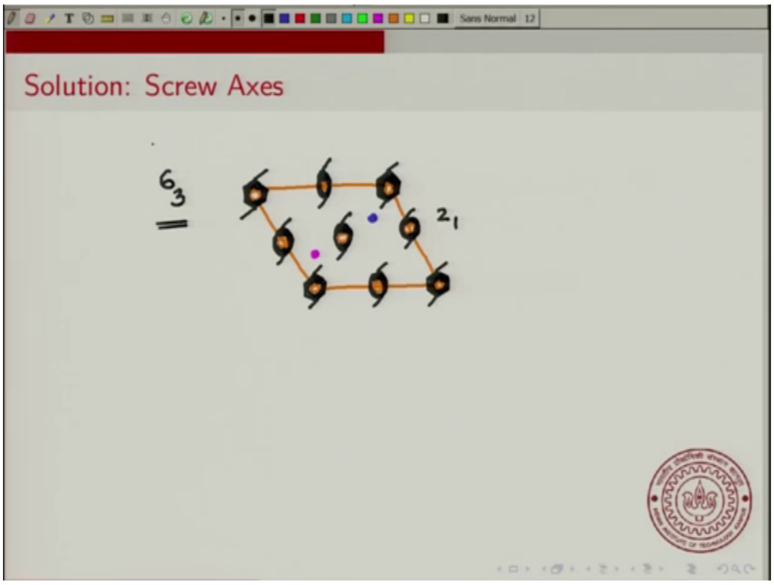

Now, what about the screw axis now it turns out that you can again work it out with this unit cell that we looked at. So, with this invertible unit cell these are all centers of inversion and you have your 2 lattice points, one was located here ,the other was located here this was one fourt and this was at three-fourth ok.

Now the screw axis in this there is a 6 fold screw axis that is located here and we want to emphasize that there is also an inversion center here in addition to the 6 fold screw axis. So, we will draw it this way and similarly it will be at all these corners. So, this is a 6 3 axis; 6 3 screw axis.

So, 3 is so that means, you rotate it by 30 degrees; rotate by 30 degrees and translate by half of the unit cell. So, if you rotate the crystal about this you can easily verify that it is a indeed a screw axis.

There are additional screw axis so for example, there is a 2 fold screw axis here right at the centre and again we want to leave the center of inversion we want to emphasize at this is also this point is also a centre of an inversion center and you have one you have other 2 fold screw axis here so these are all 2 1 axis ok.

So these are the; these are the screw axis for the diamond for the diamond cubic. So, the highest order screw axis is the 6 3 screw axis ok. But there are also this 2 1 screw axis that are there in diamond in the HCP sorry, so the highest crew axis for the HCP is this 6 3 screw axis ok.

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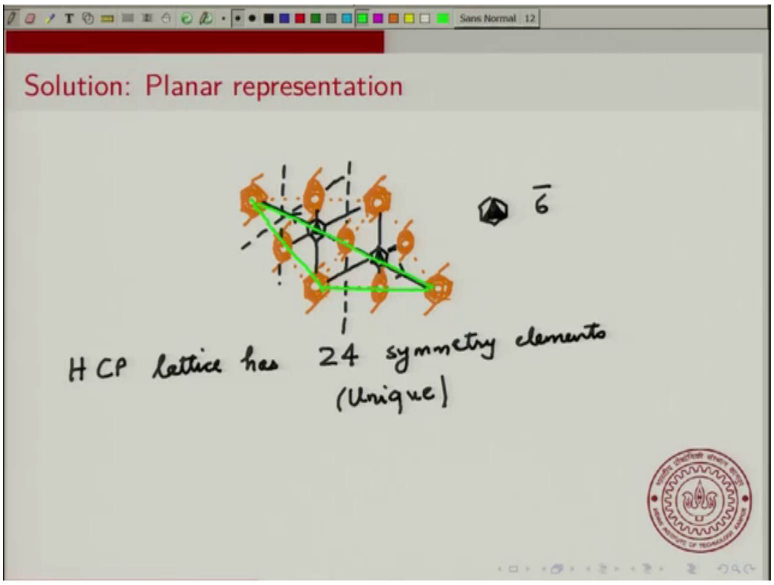

Now, let us put it all together and let us do a planar representation of the various symmetries of this HCP lattice ok, we already saw we have already seen a lot of the symmetry elements and we will just put all of it together and that is also and we had our 6 3 screw axis ok. Notice that there is a 6 3 screw axis and then inversion and therefore you have this little hole in the middle. So, we are showing both the 6 3 axis and the inversion center at this point. Similarly we will show both the 2 1 screw axis and the inversion center at this point. So, it is a 2 1 screw axis with an inversion ok, so you have the 6 3 and the 2 1 ok.

Now, let us show the other glide planes I am not going to discuss this in too much detail I will ok first I will show the mirrors. So, the mirrors the in plane the mirrors that are perpendicular to the screen are and as is the usual convention you only show the 2 fold mirrors that are perpendicular to the screen ok.

So, all these are mirrors mirror reflections and they will ok. Now there are some other interesting symmetries that are there is a 6 bar; there is a 6 bar axis right here, in 6 bar there is a symbol for 6 bar similarly there is a 6 bar right here.

So, this is a symbol for a 6 bar so and then we will show all the other. So, these solid lines are the 2 fold reflections these are the screws and we have shown a 6 bar, there are other mirrors which I will just which I will emphasize.

So for example, that is a mirror here which is actually a an in plane glide and so on you can extend it again to the entire I will have one here ok. So, this is a planar representation of not all the symmetries, but at least a significant fraction of the symmetries of the HCP cubic lattice, so HCP cubic a HCP lattice has a total of 24 symmetry elements ok.

Now the asymmetric unit of this corresponds to just one it corresponds to just 1 atom ok. So, with these 24 symmetry operations you can generate the entire HCP crystal ok. So, it has a total of 24 symmetry elements and these are the unique symmetry elements ok, unique in the sense that you only apply them to the you only look at those in the asymmetric unit. So, the asymmetric unit for instance would look like this would be an example of an asymmetric unit because it cannot be the entire cell ok.

So it would be for example, it would be this because the entire cell contains 2atoms or two points the asymmetric units will contain only one point ok. So, it will be half of this half of the entire unit cell ok. So, with this I will conclude week 4 of this course ok. So, in this week we have looked at translational symmetries and we have seen how to represent symmetries on a piece of paper or a screen.

Now I am not done these in too much detail my basic idea was I wanted to give you an idea of some of these things and these are things that you might see in various books or various websites and so it is good to know them in general ok. However, we would not be discussing too much we will not be working out too many problems in this area of symmetry and crystallography our goal is to learn how to describe crystals and then what is the chemistry of these crystals. So, with this I will conclude week 4.

Thank you.