Solid State Chemistry
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Lecture –30
Summary of Week 6, Practice Problems

Now, I will go to the last lecture of week 6 and in this lecture, I will summarize briefly what you learnt in week 6 and do some practice problems and I want to emphasize that I will just do them rather in a quick way, but you should go back and you should work them out in more detail ok. So, week 6 lecture 5, Summary of Week 6 and Practice Problems.

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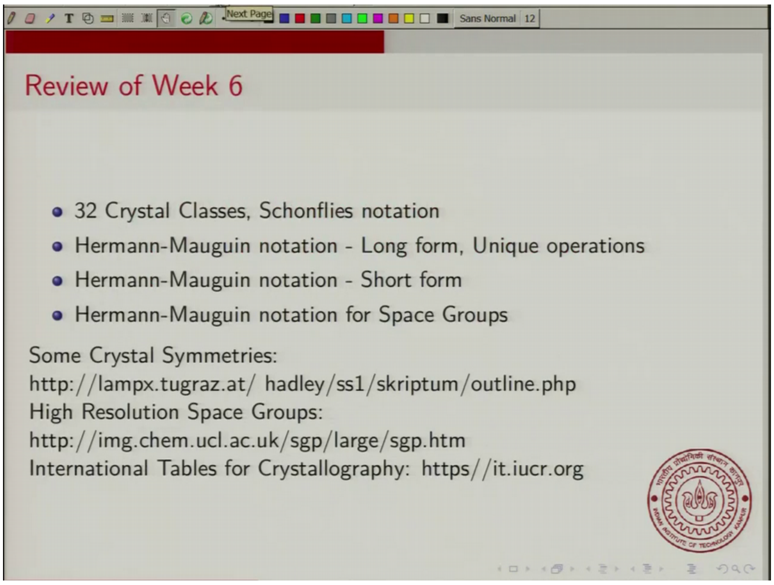

So, to summarize what you learnt in week 6, we learnt about the 32 crystal class and we learned the Schonflies notation; we learned the Hermann-Mauguin notation; we learned the long form and we learnt the concept of unique operations that was that helped us to write the Hermann-Mauguin notation. Then, we learnt about the short form of the Hermann-Mauguin notation ok, where we used lot of ideas from combination of symmetry operations and how the how combination of symmetry operations implies presence of other symmetry operations and finally, we looked at the Hermann-Mauguin notation for the space groups ok.

So, for all the 230 space groups we did not list all the 230 space groups, but essentially all these space groups have a Hermann-Mauguin notation and we briefly saw some of the features of that and again, I can emphasize that there are certain websites that which have this thing explained ok. So, this is website where they have there is a course website where one of the links talks about different crystals and it gives all the space group and the symmetry operations and then, then this is an excellent resource for getting the high the space groups at very high resolution.

So, just by giving the number of the space group, you can get the space groups at very high resolution and then there is the international tables of crystallography which unfortunately it is not a free resource, you have to purchase it ok. But it is the defining resource for lot of these details ok. So, if you have an arbitrary crystal and you have the symmetries and you want to know what space group to classify in it in then, then you can look at the international crystallography; international table of crystallography and find out the exact symmetry operations for each space group and you know check with your material and either and put it in the appropriate space group ok.

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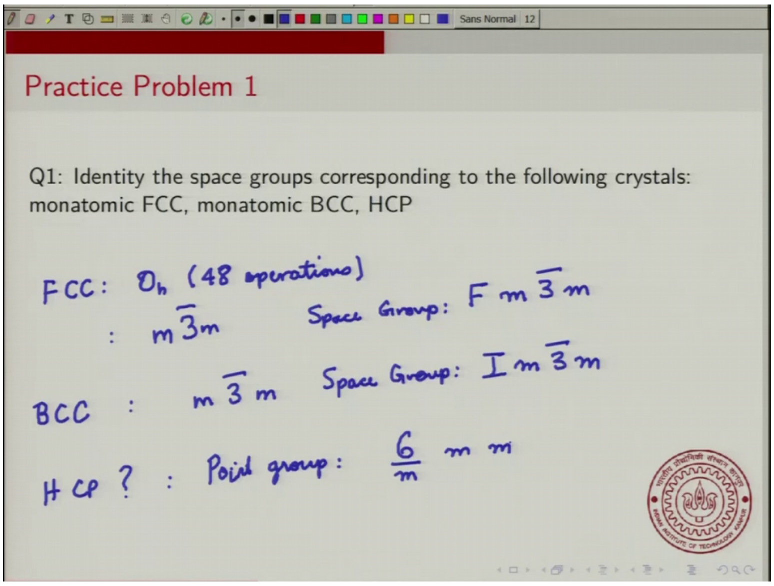

Now, let us workout a couple of fairly simple practice problems and again I encourage you to go and you know put these I mean for example, FCC, BCC, HCP. You can try to look in this in some of these resources and try to actually see what the space groups look like ok. So, identify space group for responding to the following crystals; a monatomic

FCC, monatomic BCC and then HCP crystal ok. So, let us start with the let us start with the monatomic FCC ok. Now, the short form of the point group, ok. So, the point group we already saw was octahedral with a 48 operations ok. It is a cubic crystal system and in the point group had a notation m 3 bar m.

So now, the space group in this case ok, the space group in this case is just F m 3 bar m in other words there are no additional glides or glide reflections or screw axes ok. So, the space group notation is just F m 3 bar m. What about the BCC? Now the BCC again it is m 3 bar m and there are no additional glides or screw acts screw rotations ok. So, the space group is just I m 3 bar m. Now, what about the HCP? In this case we need to inspect the point group ok. So, actually the point group is 6 by m m m. So, now, what about the space group of HCP?

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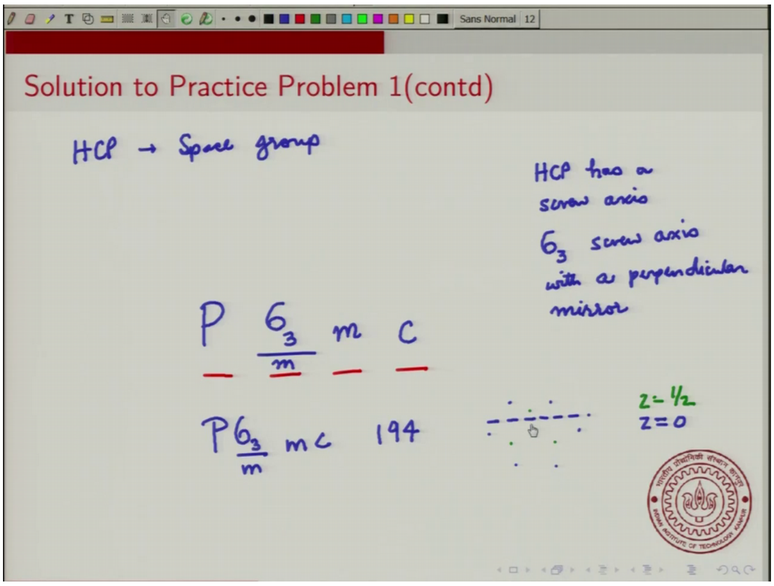

So, HCP space group ok. So, let me do this in a slightly different way. So, I will put a few. So, we have all these 4 up to a maximum of 4 symbols that we have to put. Now clearly the first one has to be primitive because in the hexagonal, we saw that only primitive is allowed ok. Now what about the 6 axis by m ok? Now we saw that in the HCP has a screw axis. In fact, it is a 6 3 screw and it has and the 6 3 screw axis has a perpendicular mirror ok. So, you have a 6 3 screw axis and a perpendicular mirror. Now the second position ok, it has to be perpendicular to the first position and it is one of the symmetry directions and this you can show is just a mirror.

Now the third position is in between the secondary mirrors ok. So, you have the 6 mirrors in the secondary that actually it will be now you will have these mirror mirrors that are that contain the 6 3 axis. And now between those mirrors, there is actually there is another mirror reflection it is not exactly a mirror reflection, but it is a c glide reflection ok. So, if you look at the hexagonal, if you look at the planar representation of the HCP ok. So, you have the hexagonal lattice and you have and you have these additional points at z equal to half. So, this is z equal to half and this is z equal to 0 and you can click you can see quite, now you can see that there will be glide reflections which will be which will be which will take one of one of the green points to one of the blue points ok.

So, there will be a c glide reflection mirrors that will be the third position ok. So, the space group of HCP is actually P 6 3 by m m c and its number if you in the crystallography table is 194. So, its number is 194 and it has a total of 24 symmetry operations which is actually the same as the I mean the if you look at the unique operations there are only 24 of them ok. So, these are the space groups of the HCP crystal. What is important?

So, the 6 3 axis was obvious, but again you can easily see that it should have a glide reflection and if you look at the third position ok, the glide reflection of interest has to be a c glide ok. Again, again it is important that there is only for the third. If you look at other positions, then you can have different glide reflections ok; you may not have a c glide ok. So, clearly if you have if you have a mirror like this that would be a c glide something like this would be a c glide plane and then, there would be equal entry there would be there would be other mirrors also ok. So, we will take we will take a mirror like this, will take this green point to the a glide reflection. So, we will take it on top of this blue point ok.

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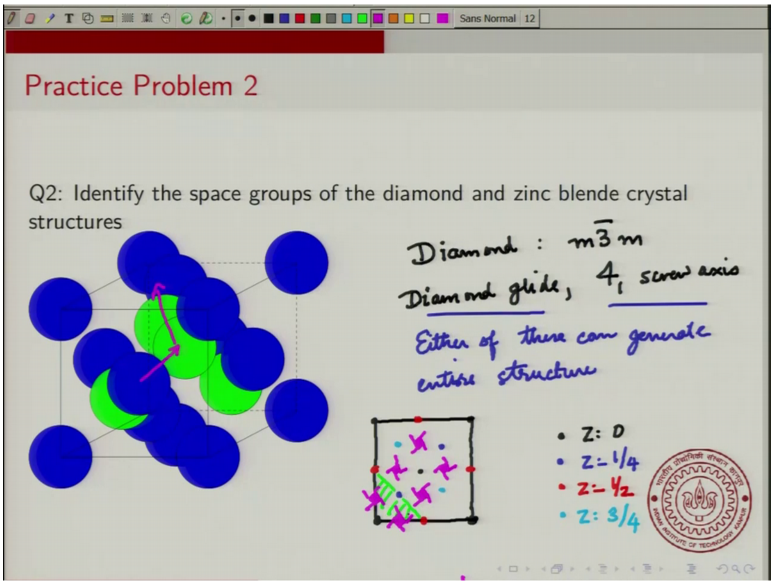

Next problem identify the space groups of the diamond and the zinc blende crystal structures. Now, this is substantially more complicated and especially the diamond. Now the point group of the diamond crystal is the following ok. So, we will start with diamond ok. Now this is in the m 3 bar m ok. So, that is the cubic system and the hexoctahedral class crystal class and if you in addition to these ok, we notice that I mean in case of diamond the, there is a die diamond glide and a 4 1 screw axis ok.

So, these are the 2 translational symmetry elements that are there in the diamond crystal ok. You recall is a point to recall is that is that either of these either the diamond glide or the screw axis ok. These can generate the entire crystal. So, both the diamond; so, either of these can generate entire structure and to see this ok. So, we saw this when we were doing the when we are seeing the screw axis, we saw that if you if you if you imagine the if you look at the diamond cubic structure in the planar representation and I will take the coming I mean I will show the I will show the entire cube ok.

And you imagine that you have point set. So, this is z equal to 0. Then, you have point set z equal to 1 by 4; z equal to half and finally, at and now we know very well that there is a screw axis of rotation ok. In fact, in fact there are several screw axis of rotation and you can you can show for example, you can you can easily show that there is a 4 1 screw axis that passes through this point ok. Let me show it in a different color. So, this is a 4 1 screw axis ok. So, we have this 4 1 screw axis and similarly you have several others flow axis in diamond ok. Now, what we said is that if you take this 4 1 screw axis ok.

So, this is actually a 4 1 screw axis. So, what it will do is it will take if you operate once by this 4 1 screw axis, then this black point will go to the light blue point which is at a higher. So, it corresponds to rotation by 90 degrees and then it will be raised by one-fourth ok. So, it will come to this point and you can go ahead and you can do this and then the next time it will come on top of this and this and so on ok. What you can show is that if I show it on this big figure and let me use a slightly different; let me use this purple color. So, this was that point in black and if you if you do one of these screw operations. So, you have a 4 1 screw axis here and what this 4 1 screw axis will do is it will take this point at z equal to half rotate by 90 degrees and raise by one-fourth.

So, it will come here and what you can see will happen is that is that this blue point will go to this green point now. In fact, in fact, what I am showing is something slightly different; I am showing this blue point will go to this green point and if you again, if you again put if you again apply this screw rotation ok; then, you will see that you will end up at this point and this will this will keep going on ok. Now there are other screw axis also in the crystal. So, there is a 4 1 screw that is there here ok. This will also generate the remaining points ok. So, what you see is that if you have a 4 1 screw ok, then this mirror ok; then, you can generate the all the other points ok. So, by operating this 4 1 screw multiple times you will find that you can generate all the required lattice points ok.

Now, again there will be a 4 3 screw here and another 4 3 screw here ok, but you keep in mind that the asymmetric unit of diamond; diamond has 8 atoms in the crystal. So, this asymmetric unit we only need to consider one of these one of these has your asymmetric unit ok. So, you can just take one one-eighth of this of this of this cube for the asymmetric unit. So, for example, you could take you could take this as the asymmetric unit and now we will have to put the other screw axis here and here ok. So, with this screw axis we can generate the other points in this asymmetric unit ok. So, similarly the glide plane can also be used to generate several other symmetries in the several other points ok.

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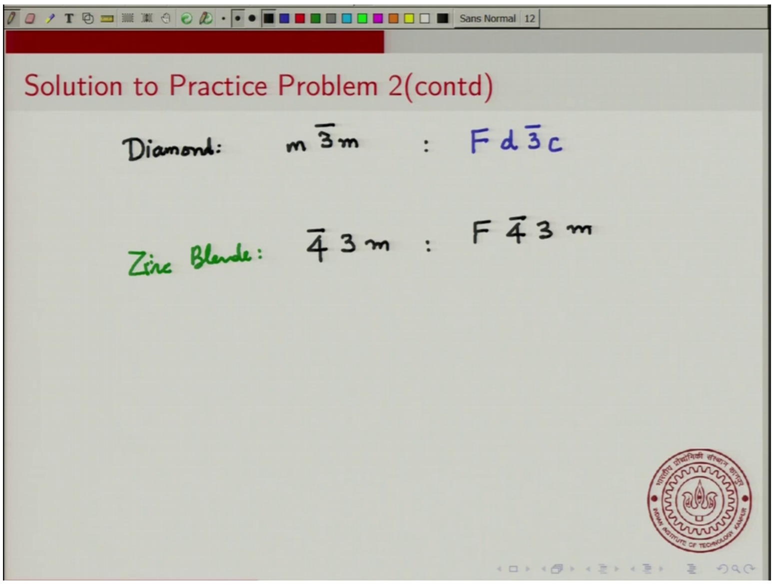

So, to make the long story short ok, we will say that in diamond you have an m 3 bar m ok. This is the point group ok. Now clearly it is the space group ok. Since it is face centered, you have an F here and now the first the first space you can have a you have a 4 1 screw axis, but we saw that the 4 fold axis is a consequence of the 2 mirrors ok. So, and what we can do is that you still have to have the 3 bar ok. Now, if the third mirror is actually a glide mirror. And now because you have the glide the glide will generate the 4 1 axis ok. So, but there is an additional operation that is the diagonal glide ok.

So, actually the first position corresponds to the diagonal glide then you have the 3 bar and then, you have the c glide ok. So, these 3 will generate the space group of diamond ok. Now what about Zinc blende? Now, in this case in this case you do not have the full symmetry of the cube. In fact, the point group is 4 bar 3 m and in this case the space group ok; space group again it is face centered it is just 4 bar 3 m. So, there are no glide operations or no screw axis ok.

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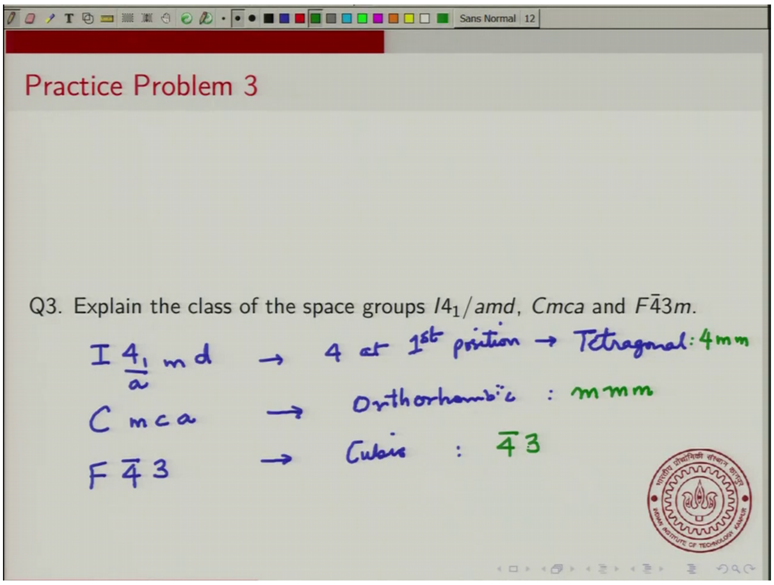

So, one more example and then we will conclude this week ok. So, this is explained the class of the space groups and I have given 3 space groups. I have called 1 I 4 1 by am 4 1 by amd, Cmca and F 4 bar 3 m. So, identify this I identify the class of these space groups. So, clearly now let us look at each of them. So, we look at I 4 and subscript 1 by amd ok. Now, the 4 at the first position implies ok. So, this could mean either cubic or tetragonal in this particular case ok.

So, you have an a glide and a d glide and you have a 4 1 ok. So, we saw that in the cubic this you can never have this kind of combination. So, this is actually tetragonal ok. So, in a cubic if you the middle index has to be 3 bar ok. So, you cannot have an m here; the 4 at first position implies either cubic or tetragonal. So, this has to be tetragonal. Similarly if you look at Cmca ok, now there are 3 mirrors ok. So, there are 3 mirrors and you can have a c centered. So, this has to be orthorhombic ok. The, what I should say is the crystal system. So, the crystal system is orthorhombic the crystal class is mca. This is the crystal classes just for actually the crystal classes mmm; crystal classes mmm.

Here the crystal class is 4 mm ok. Now the last case you have F 4 bar 3 and here this is since you have a 3 at the second position, it has to be cubic and the crystal class here is just 4 bar 3 ok. So, this is the crystal class ok. So, with this I will conclude week 6 of this course ok. So, what you see is that from the space group notation, you can say when you can at least identify the crystal system and you can say whether it is face centered, body centered or you know what kind of centering it has. So, this information at least you should be able to identify given the space group ok.

Now, the other details of you know which exactly which crystal class it belongs to or exactly which what is the what are the details of the space group that is much harder and that is you typically we refer to the tables to find that out ok. But at least the basic crystal system and whether it is and the centering should be easy to infer from the name of the Hermann-Mauguin symbol for the space group ok. So, I will conclude week 6 here and then, in the next week, we will start talking about defects in crystals.

Thank you.