

CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 28: Derivation of the Remaining Plane Groups

We have so far discussed a total of 13 plane groups in which we had utilized all the point groups to be incorporated in the different two-dimensional lattices. But there are a few more possibilities and let us consider what are those few more possibilities. We could replace the mirror with a glide.

Let us see how I could do this. Consider a primitive rectangular cell and to this we add a glide plane. So, this can quite easily be done like this. So, I have let us say this is my primitive rectangular net and instead of putting a mirror along the cell edge, I can add a glide along this edge.

The lattice translations \bar{a} and \bar{b} and the lattice translation \bar{b} will take this glide plane to the other cell edge and also the result. So, if I call this as G the result of reflection followed by translation \bar{b} would give me another (in fact, not reflection but glide) plane σ'_{τ} and its location is going to be exactly midway just like it will operate just like the mirror.

$$\bar{b} * \sigma_{\tau} = \sigma'_{\tau}$$

One could very easily see this. If I put let us say a right-handed motif the glide would reflect it and then go through a glide translation τ and the motif would come here and it will become left-handed. The translations will take these two motifs out here and out here.

So, if I call this as motif 1, motif 2 and then the translation takes it. So, this is perhaps not the correct location, it would be a little bit more down and it would be somewhere here and therefore, this is motif number 2 and then the translation takes it to motif number 3.

Now, how is motif 1 related to motif 3? It is related through a glide right in the center, as you can see the handedness changes. Similarly, if I call this as motif 4, then motif 4 and 2 are also related to each other by the same glide in the middle of the cell.

So, this particular, so this is a valid plane group, it will follow all the rules of the group and this motif is simply called as instead of pm if you recall this motif is called pg . In the earlier motif pm these glides are replaced by mirrors. So, that is what we have done; we have simply essentially replaced the mirrors with glides.

Now, since I could do this to the plane group pm I could do this also to the plane group cm after all what was my plane group cm . My plane group cm recall again it is a centered rectangular lattice this time and I add a mirror. Mirror along this, there will be a mirror here, there will be a mirror here, but because it is a centered group and there is a centering translation, because of this I get glide planes at these locations between the pairs of mirrors. This is the plane group cm .

Now what about it if I started with the glide instead of adding the mirror. I do the following: I add this time on the cell edge a glide. Naturally because of the lattice translation \bar{b} , I will get a glide plane in the middle and obviously I will also get the glide plane at the other edge.

Now what else can I get in this? Again, remember this has a centering translation. Let us call this translation as the vector t and this is I will denote this as glide g .

So, now I do a glide operation σ_τ for this glide plane g . But then what will be the value of τ ? The value of τ would be half the lattice translation along the glide plane. Now, the full lattice translation along the glide plane is a and therefore, τ would be $a/2$. So, instead of writing it as τ let me write this as $a/2$.

$$t * \sigma_{a/2}$$

Follow this translation or follow this glide operation perform the lattice translation T , which is the centering translation. Now, as before, let us break this into a perpendicular component and the parallel component. So, the parallel component, so this is my parallel component and this would be my perpendicular component.

All I have done is I have represented \bar{t} as $t_{\parallel} + t_{\perp}$. ($\bar{t} = t_{\parallel} + t_{\perp}$)

Now, what would happen as a result of this? So, let us try this. What should happen? Well, let us say that actually I should get another glide and let me call that as $\sigma_{\tau'}$. I just have to figure out what my glide translation is in this case.

$$\bar{t} * \sigma_{\frac{a}{2}} = \sigma_{\tau'}$$

So, τ' should be equal to previous τ which was $a/2$, plus an additional translation which would be t_{\parallel} . Now, what is t_{\parallel} ? Well, t_{\parallel} is clearly $a/2$.

So, I have $a/2 + a/2$ and my new glide translation becomes a .

$$\tau' = a$$

But then a is a lattice translation and we have seen this in an earlier lecture that if the glide translation becomes a lattice translation, then it is no longer a glide plane, but it is actually simply a mirror plane and therefore, in between the two glides I will get mirrors.

Now, compare these two diagrams. What do you see in this basically we see the same set of symmetry elements distributed in exactly the same way only difference being that the cell has been offset by one quarter along the translation \bar{b} . So, they are essentially both of them identical and hence we will find that there is no cg plane group mentioned. So, even if we were to call it as cg it is actually cm .

So, cg equals cm and cm is the conventional notation that one uses. So, therefore, it is not that if I keep adding I will keep getting more and more plane groups. We may end up

getting the same plane groups and, in some cases, it will not even be possible to add or replace a mirror with a glide plane. So, I should say that this is not there.

Now, we do one more thing. How about replacing one of the mirrors in $p2mm$. So, we start with the plane group $p2mm$ and we replaced one of the mirrors with a glide plane.

So, first let me just sketch out the plane group $p2mm$. The $p2mm$ if you recall or you can simply go back to the previous lectures, I will have 2-fold rotational symmetries at the corners, in the centers of all the four edges and in the center of the cell and mirrors will be running horizontally and vertically.

Now, I am going to replace one of the mirror planes with a glide. So, let me sketch this figure again and this is how we are going to do it. What we will do is start with the plane group $p2$. So, there are no mirrors added right now and let me add glide planes in a vertical orientation. I can also do it horizontally.

So, if I put it here, the translations will put glide planes at these locations as well. Now, let us try to figure out this is g . Let us try to figure out the glide σ_{τ} followed up with a rotation of 180° due to the two-fold rotational symmetries.

So, if I at this particular point for example, there would be a top corner which would have a rotational rotation of 180° , so a π . And we want to find out what is the resulting symmetry operation as a result of this combination.

Let us do this geometrically. You start with the right-handed motif let us call it 1, 180° rotation will bring the motif at position 2 without changing the handedness. Next what we do is operate the glide. If I operate the glide plane on the motif number 2, what would happen is there will be, let us say, a translation followed up with reflection and I will get motif number 3 which is left-handed. And of course, the lattice translations will take these motifs everywhere else, but let us just focus on this.

So, I am going from 1 to 2 through the rotation of π and 2 to 3 as a result of glide. Now, I want to find out how to go from 1 to 3. Well, both of them as you can see have different handedness: one is right-handed and the other is left-handed. So, what kind of operation will take me from 1 to 3 which changes the handedness? And as you can very clearly see from this geometry that it has to be a mirror and clearly the location of the mirror has to be here.

So, this becomes one of the mirrors and of course, other translations will take the mirror here as well. And this becomes the complete plane group which is not the same as $p2mm$

Now, here if I just look at this, if I let other operations take place, for example, take 3, 180° rotation around this particular axis will bring it here, then the mirror will reflect it here, then another 180° rotation will bring the motif here and right-handed. The translations: so 2 will travel to this position, similarly 1 will come here, 3 as a result of translation would be here and other translations as you can see would put the motifs here and here.

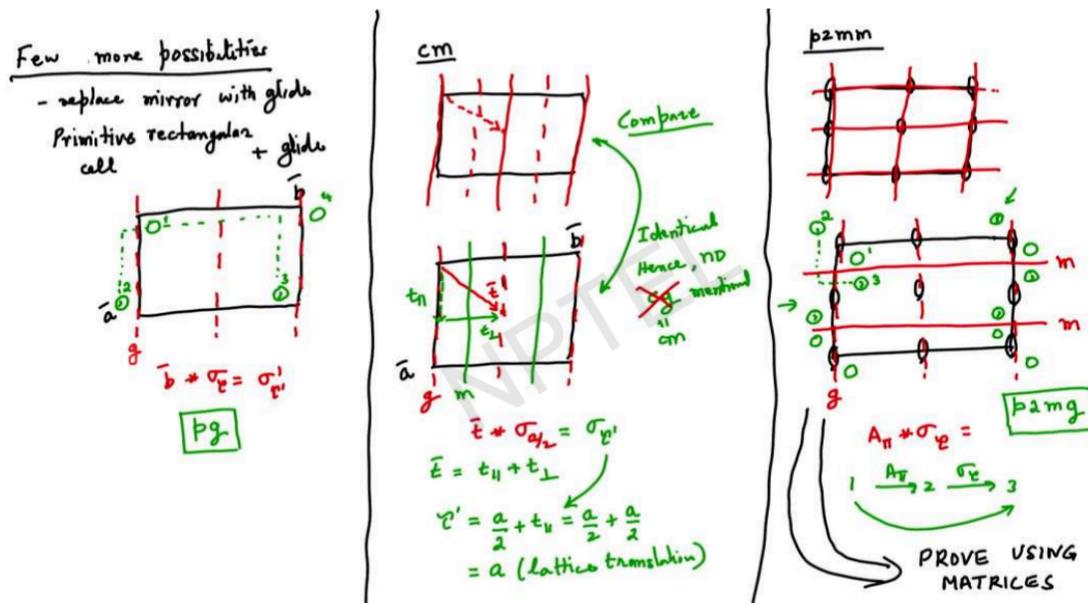
So, this is the complete plane group with the motifs drawn in them. This particular plane group we will call it as $p2mg$. So, one of the mirrors has been replaced by a glide plane. And the methodology for notation we have discussed in the last lecture. Apply this methodology to this. I will leave this to you so that it conforms to the notation system.

Now, one can also prove this, and this also I will leave to you, to prove the resulting horizontal mirror using matrices.

So, we have developed two more plane groups. So, we had 13, now we have reached the number of 15.

Can we do something else? Let us try and figure that out. What we can do is *Interleaving of symmetry planes*. So, what does this mean?

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Let us start with the plane group $p2mm$ again. Two-folds. So, what I do in this case, I try to put a glide plane. So, this is basically the plane group $p2$. And I am not adding the mirror planes; I am only going to add the glide plane, but in a different way. I am going to add the glide plane in between the rotational symmetry. So, they are not going to pass through the two-folds, but I have to add them in such a way that I do not end up wrecking the symmetry.

What that means is that the glide plane should operate on the two-folds, but then they should fall in a location where there is also another two-fold. How can I do this? I can suppose I put the glide plane out here. What will happen? This rotational symmetry will get reflected across the glide plane and then translated. So, it will go like this and then translated, falling on top of the other two-fold. So, therefore, I am not generating any new two-fold symmetry.

So, this is an allowed position that I can have for this glide plane. Very clearly, I do not have to explain, there will obviously be another glide plane coming out here. Are there going to be other things in this? Well, let me start with the right-handed motif. 180°

rotation takes it here and this particular glide plane will reflect, bring it here. Rather, I first reflect it across here and then I translate it.

So, where will this go? This will go all the way out here somewhere, and I will do a glide translation and bring it to this position. Have I done this correct? I think I might have made a mistake. This is not right. This will simply come somewhere below here and then lattice translation will bring it out here. This is location number 3.

So, 1 to 2, then 2 to 3. How do I go from 1 to 3? I think that is easy to see: there would be a vertical glide plane showing up here. Now, similarly, there will be another vertical glide plane showing up here. So, this becomes a new plane group and I will call this. You can also try other motifs putting in to make sure that this is correct. This is labeled as $p2gg$. There are no mirror planes here. Now, this is the sixteenth plane group we have.

How about doing something with the plane group which has a fourfold rotational symmetry? So, let us draw this. Let us first draw the $p4$. So, I have fourfold rotational symmetries at the corners and I will have one in the center and I will have two-folds in the center of the edges.

This time let me try to add a mirror plane in a different way. In the $p4mm$ the mirror planes are added along the cell edges and the translation symmetries will take those mirror planes everywhere else. But here, how can I add another kind of interleaving between the axes?

If I want to add a mirror plane here, well this is not going to work because this fourfold will get reflected on top of the twofold. So, that would end up creating another rotational symmetry. In fact, the entire symmetry of the square lattice will be wrecked.

What I can do is I can put a mirror plane in this fashion. Here, now the fourfold will reflect on top of the four-fold. Very clearly it is not going to create any problems in putting it like this. The central four-fold will take this mirror like this and you can see that it is not going to create any problems with the rotational symmetries lying elsewhere.

Now, what can I figure out from this? Well, you can take one of the mirrors and look at a translation. So, I can take for example this mirror and this translation. What will this do? I break this translation into a parallel component and a perpendicular component. Clearly, these four mirrors make a square. So, the parallel component is this and the perpendicular component is this one.

So, this is T_{\perp} and this is T_{\parallel} . And therefore, there will be a glide plane that will show up at the midpoint of the perpendicular component and parallel to the mirror plane. Now, similarly there would be a glide plane along the other diagonal. So, these are all glides.

Are there any other glides? Yes, there are. And in order to figure that out, what I could try to do is: let me add a right-handed motif, call it 1, give it a 90° rotation. The right-handed motif moves to another right-handed motif at position number 2. And then what else can happen?

What actually can happen is that motif number 2, this particular glide plane operates on it, it reflects and brings it out here and the handedness gets changed to left-handed. Now, how do I go from 1 to 3? Well, 1 to 3 will be another glide which will be a vertical glide. Now, this central fourfold will take this glide and produce these extra glides.

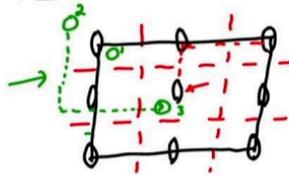
So, this is a complete plane group that I have drawn. Let me just draw this in a separate diagram. This diagram is a little cluttered now. So, I have fourfolds and the twofolds and then I put the mirrors and then I put the diagonal glides, the vertical glides, and the horizontal glides making the complete plane group which is labeled as $p4gm$ and you can compare this notation with the methodology I have given and see that this is indeed correct.

Now, in fact if I try to add, let us say, interleaving symmetry planes inside the hexagonal-based plane groups, they could be put interleaving glide planes in those lattices as well, but they are not going to create any new plane group.

So, in fact that is all. We finally come to an end and to sum it up, if I add up all the plane

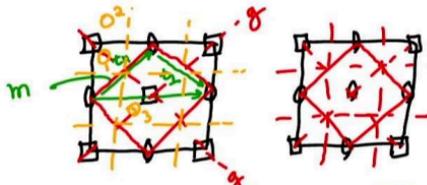
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Interleaving of symmetry planes



pgg

TOTAL OF
17 PLANE GROUPS

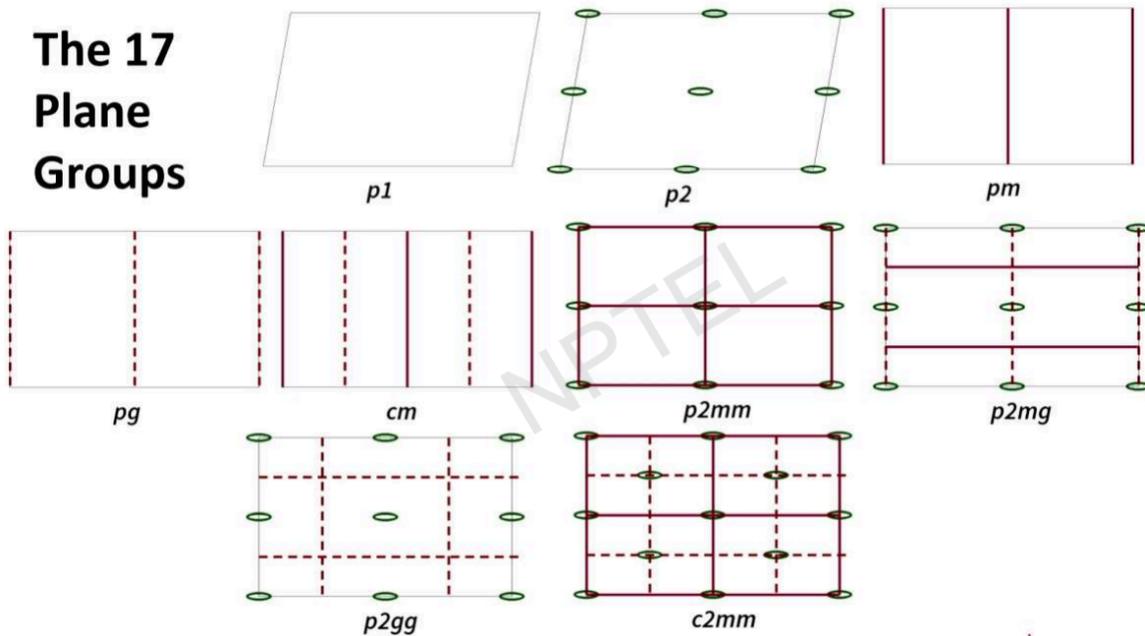


$ptgm$

groups, we have a total of 17 plane groups, there are no more and no less. And just to conclude this lecture, let me show you all the 17 plane groups.

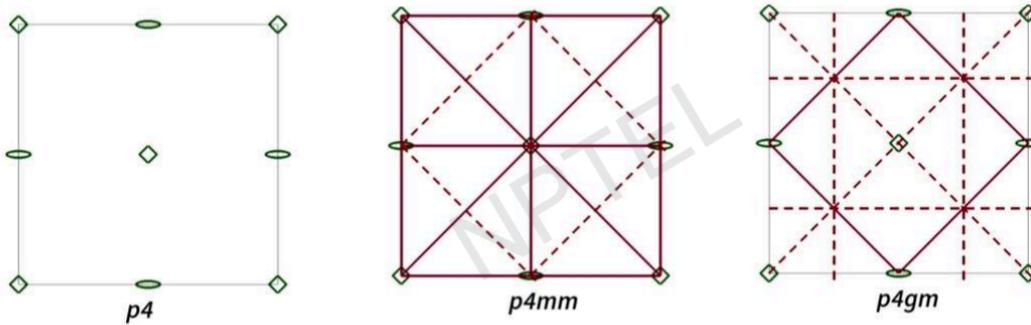
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The 17 Plane Groups

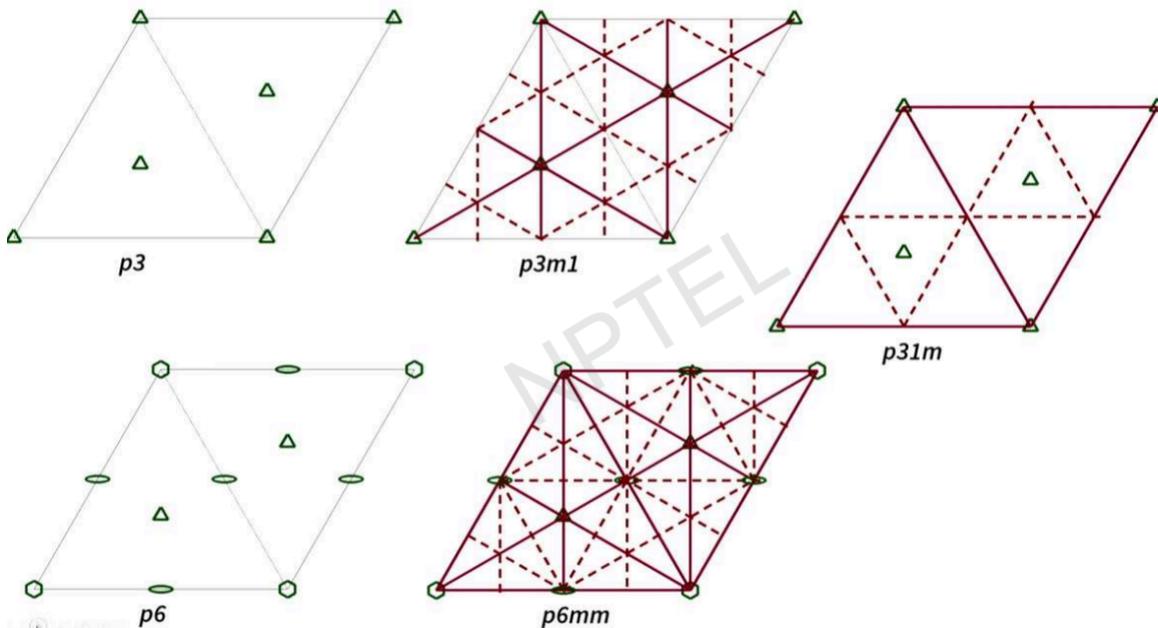


So, here we have $p1$, $p2$, pm , pg , cm , $p2mm$, $p2mg$, $p2gg$, $c2mm$. So, we have 9 plane groups; here we have 3 more that makes it 12 based on the fourfold rotational symmetries; and then we have 5 more making it a total of 17 plane groups.

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Now, I conclude this lecture here. In the next lecture we will look at one small topic in which I will introduce what are called the international tables for crystallography.