CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 27: Hexagonal Plane Groups based on the Point Symmetry 3m

In the last lecture we were discussing plane groups formed by the hexagonal two-dimensional lattice. This is where we were. Here we have a primitive hexagonal lattice to which the point group $3m$ is added. There are two possibilities for placing this point group on the lattice.

One possibility is to place the mirror planes along the cell edges. So, one mirror plane is along the edge, another along the next edge, and the third is along the short diagonal of the cell. This is the case we considered earlier. To repeat that part:

Consider the mirror plane M_1 on the short diagonal. Take the reflection σ_1 across this mirror and follow it with a lattice translation. The lattice translations are $\bar{a}$ and $\bar{b}$ along the two edges. Suppose we apply σ_1 followed by $\bar{a}$. Because this translation is at an angle to the mirror, we expect a glide plane.

To find the glide, break the translation vector $\bar{a}$ into two components: one parallel to the mirror, $T_{||}$, and the other perpendicular to the mirror, $T_{\perp}$. Here $T_{||}$ is exactly half the lattice translation along that direction because the midpoint lies halfway along the diagonal.

The result of σ_1 followed by $\bar{a}$ is a glide reflection σ_τ where the glide vector $\tau = T_{||}$. The glide plane lies at the midpoint of the perpendicular component, i.e. at $T_{\perp}/2$. This gives the glide plane G_1.

$$\bar{a} * \sigma_1 = \sigma_{\tau=T_{||}} @T_{\perp}/2$$

Now consider another mirror, say M_2, along a cell edge. Take the reflection σ_2 and follow it with the diagonal translation vector $\bar{t}$ (from one corner to the opposite one). Decompose $\bar{t}$ into $T'_{\parallel}$ (parallel to M_2) and $T'_{\perp}$ (perpendicular). Here $T'_{\parallel}$ again ends at the midpoint, while $T'_{\perp}$ reaches the opposite lattice point. The combination σ_2 followed by $\bar{t}$ again gives a glide σ_{τ} with $\tau = T'_{\parallel}$. The glide plane is located at $T'_{\perp}/2$. This gives the glide G_2.

$$\bar{t} * \sigma_2 = \sigma_{\tau=T_{\parallel}} \; @T_{\perp}/2$$

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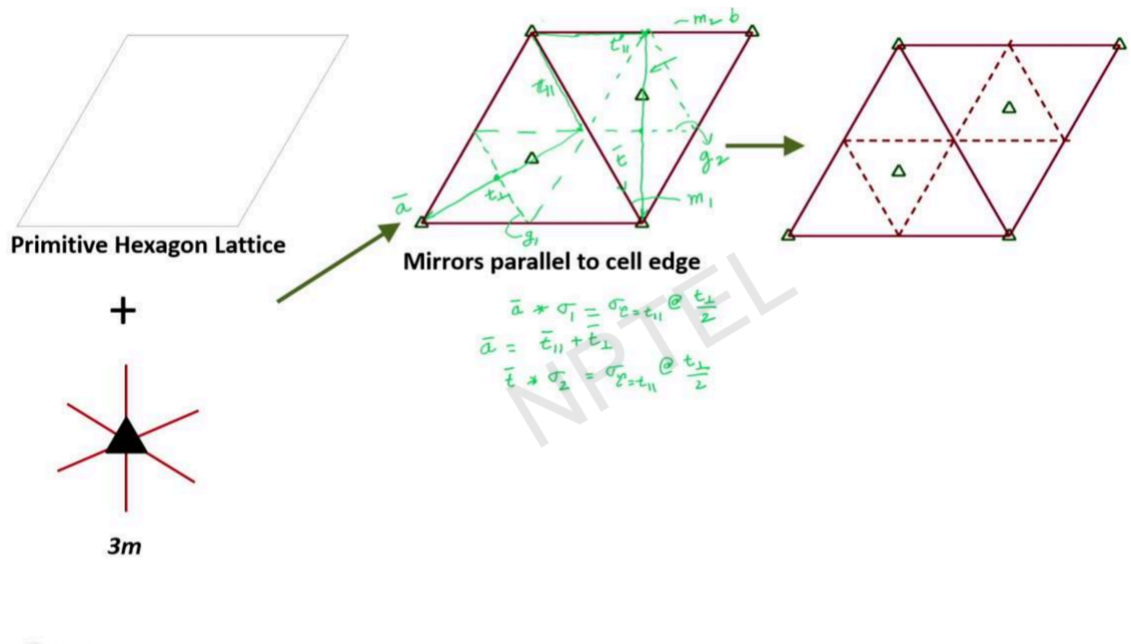

All other glides appear from symmetry operations. By completing this construction, we obtain the full set of glide planes for the case where the mirrors lie along the cell edges.

Now consider the second orientation of the point group $3m$. In this case, the mirrors are placed perpendicular to the cell edges. The diagram is redrawn with the mirrors positioned so that each one is perpendicular to an edge. Let us call one of these mirrors M_1.

We repeat the same procedure. Take σ_1 across M_1 and follow it with a lattice translation (for example $\bar{a}$, $\bar{b}$, or the diagonal translation $\bar{t}$). Decompose the translation into $T_{||}$ and $T_{\perp}$ relative to M_1. The combined operation again gives a glide reflection with glide vector equal to the parallel component and positioned at the midpoint of the perpendicular component. Doing this for all mirrors and translations produces the complete set of glide planes for this second orientation.

Thus, the two different orientations of the $3m$ point group. The mirrors along the cell edges and the mirrors perpendicular to the cell edges lead to two different plane-group patterns, each with its own arrangement of glide planes.

Now let us look at a particular operation. Take the reflection operation σ_1 across mirror 1 and follow it with the translation vector $\bar{a}$. The translation vectors here are $\bar{a}$ and $\bar{b}$. Consider the vector $\bar{a}$. This vector can be broken into two components. The parallel component is along the mirror, and the perpendicular component is along one of the cell edges, $T_{\perp}$. Immediately we can see that the glide plane should appear at the midpoint of this perpendicular component and parallel to mirror M_1. This is the position of the glide.

Now we check whether $T_{||}$ is exactly half the translation vector in that direction. Draw two adjacent hexagonal cells. The component $T_{||}$ does not end at a lattice point, but if extended further it ends at the lattice point in the next unit cell. It therefore connects one corner of a cell to the corresponding corner of the adjacent cell. Clearly $T_{||}$ is half of that lattice translation. Hence the operation produces a glide G_1, i.e. σ_{τ} where $\tau = T_{||}$, located at half of the perpendicular component.

Now take the reflection σ_1 again and this time follow it with the translation along the short diagonal, which we call $\bar{t}$. The parallel component is the same as before. The perpendicular component, $T'_{\perp}$, is opposite to the earlier one. The glide plane will again be parallel to the mirror and at the midpoint of this perpendicular component, giving another glide plane.

Next consider the situation where the mirror plane is along the long body diagonal. Complete the earlier case: σ_1 followed by $\bar{t}$ produces another glide. Now take σ_2 followed by the translation vector $\bar{b}$. Break $\bar{b}$ into a parallel component $T''_{\parallel}$ and a perpendicular component $T''_{\perp}$. Again, the glide plane will appear parallel to mirror 2 in the corresponding position.

By symmetry you can now fill in all the remaining glide planes. After removing the clutter, the complete set of glides in the cell appears. We have glide G_1, glide G_2, and glide G_3, with the rest generated by symmetry.

Thus, we obtain two plane groups based on the primitive hexagonal lattice and the point group $3m$, simply by changing the orientation of the mirrors. No other orientations are possible. These are the only two plane groups we obtain.

The notation now presents a problem. Earlier we simply used p or c followed by the point group. But here that would give $p3m$ for both, and we need to distinguish them. Therefore, the notation is $p31m$ and $p3m1$.

This needs some explanation. There is a longer, general notation for plane groups, consisting of four symbols. We place four placeholders. The first symbol is p or c: p for primitive, c for centered. If the notation starts with c, then it must be a centered rectangular lattice. If it is p, then it is one of the other primitive lattices, which can be identified from the remaining symbols.

The second symbol indicates the highest rotational symmetry. The third symbol indicates the symmetry perpendicular to the x-axis (or the a-axis). The fourth symbol indicates the symmetry at an angle α to the x-axis (or to the a-axis).

So, let us now look at $p31m$ and $p3m1$. First of all, p stands for primitive, and the highest rotational symmetry is the threefold rotation symmetry. That is the second symbol. Then we have the 1 in the top figure. This is the third symbol, a symmetry perpendicular to the x-axis or the a-axis. In this case we do not have any symmetry there. The second and third symbols are always either a glide plane or a mirror plane.

So, a 1 means no mirror plane and no glide plane perpendicular to that axis, which corresponds to one-fold symmetry or no symmetry. Therefore, the third symbol becomes 1. The last symbol can again be a mirror plane or a glide plane at an angle. So, we put m there. The mirrors are at some angle α; this angle could be 0°, 90°, 60°, or 45°. That is how the symbol $p31m$ is obtained.

Now consider the second plane group $p3m1$. Again $p3$ is clear: primitive with threefold rotational symmetry as the second symbol. The third symbol is m. This is the symmetry perpendicular to the x-axis. In this case the orientation of the point group is such that the mirrors are perpendicular to both the x- and y-axes. So, a mirror goes as the third symbol, and there is no symmetry to put in the fourth symbol. Therefore, the notation becomes $p3m1$. With this we have these two plane groups completed.

We have still not looked at one plane group. We have taken care of all the point groups so far out of those ten groups, but we have not looked at $6mm$. We now add $6mm$ to the primitive hexagonal lattice. This is an interesting one. I have put all the mirrors of the point group $6mm$ into this diagram.

You can see the six-fold rotational axes at the corners, the two-fold rotational symmetries at the centers of the edges and at the center of the cell. If you want to know how the twofold symmetries appeared, you can go back to the lecture where I discussed adding the point group 6 to the hexagonal cell. We also have the two three-folds inside the cell at the centroids of the two equilateral triangles.

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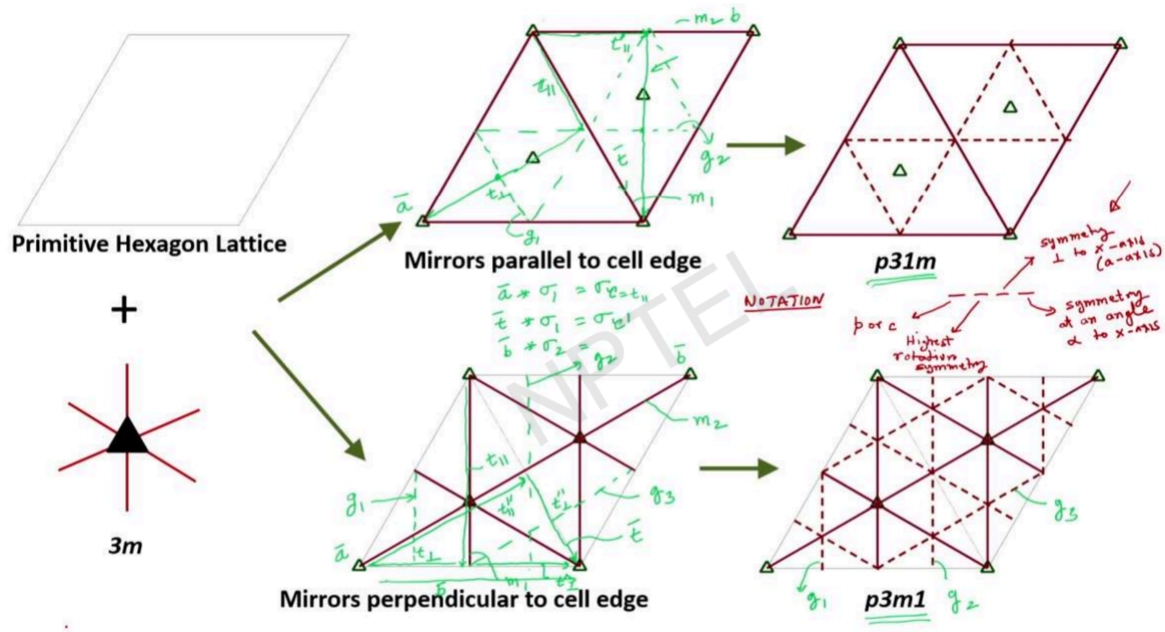

Looking at this, it is natural to expect many glide planes. But actually, it turns out to be simple because we have already done the two plane groups $p3m1$ and $p31m$. Let us look at them again. In $p31m$, the mirrors were placed along the cell edges. In $p3m1$, the mirrors were placed perpendicular to the cell edges.

In the case of $6mm$, we have many more mirrors: mirrors along the cell edges, mirrors parallel to the cell edges, and mirrors perpendicular to the cell edges as well. Essentially if we superpose both plane groups $p31m$ and $p3m1$ on the diagram of the $p6$ plane group, we get exactly the same mirrors, both sets superposed. Therefore, logically, the glide planes also get superposed. Once all the glide planes are added, we obtain the plane group $p6mm$.

There is a lot of symmetry in this diagram: many mirrors and many glide planes forming the plane group $p6mm$. When motifs are placed, they will also move around according to all these symmetries, forming an intricate pattern.

So far, counting all the plane groups I have covered in the last few lectures including this one, I find that I have done thirteen plane groups. But is that all? I have exhausted all the point groups and added them to the five lattices in all possible ways. At first glance it may appear that these thirteen plane groups are all there is.

But there are still a few more possibilities. We will discuss these possibilities in the next lecture. I will close this lecture here and begin the next one by considering all the possibilities and arriving at the complete set of plane groups.

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