CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 24: Plane Groups-I

In this lecture, we derive the various plane groups based on the two-dimensional lattices and their compatible point symmetry operations.

We already have the 2D lattices and the point groups associated with them. There are 5 2D lattices and 10 2D point groups. Combining them produces plane groups.

- Primitive oblique lattice can accommodate point groups 1 and 2.
- Primitive rectangular and centered rectangular lattices can accommodate m and $2mm$.
- Primitive square lattice can accommodate 4 and $4mm$.
- Hexagonal lattice can accommodate 3, m, 6, and $6mm$.

Adding point groups to these lattices directly gives 12 plane groups, though more plane groups emerge from combinations.

Let $\overline{a}$ and $\overline{b}$ define the oblique lattice vectors.

Point group 1 adds no symmetry beyond the lattice translations. Any asymmetric motif placed at a lattice point will be translated along $\overline{a}$ and $\overline{b}$, generating copies at all lattice points. This plane group has only translation symmetry.

Point group 2 adds a two-fold rotation. Place the two-fold rotation at a lattice point (corner). Translation generates two-fold rotations at all other corners. Combining two-fold rotation with translation generates new two-fold axes along the edges and diagonal of the unit cell: two-fold at edge centers and two-fold at the center of the diagonal. Each 180° rotation of a motif produces a new motif, and translations propagate them across the lattice.

The primitive square lattice can accommodate 4 *and* $4mm$. Place a four-fold rotation at the corners. By the principle of rotation plus translation, additional four-fold rotations appear on the perpendicular bisectors of translation vectors, at a distance of $T/2$ from the original axis.

Since 180° rotation (two-fold) is a subset of four-fold rotation, two-fold axes also appear on the edge centers. A motif placed at one lattice point evolves as follows: rotate 90° about the corner; another 90° rotation; after four rotations, translations replicate all motifs throughout the lattice.

In a hexagonal lattice, $A = B$ *and* $\alpha = 120^{\circ}$. Adding a three-fold rotation at the corners places a 3-fold axis at each corner. Combining three-fold rotation with translations, additional three-fold axes appear along the perpendicular bisector at a distance:

$$d = \frac{T}{2\sqrt{3}}$$

Translating along the lattice vector b propagates the three-fold axes throughout the lattice. We can divide the cell into two equilateral triangles; the perpendicular bisector distance takes us exactly to the centroid of the triangle, so a three-fold appears there. Similarly, another three-fold appears symmetrically. This completes the symmetry diagram for this plane group. Motifs can then be placed and transferred by translations.

For hexagonal lattice plus point group 6 (6-fold rotation symmetry), again $A = B$ and $\alpha = 120^{\circ}$. Place a 6-fold at the corners. Adding a translation vector and performing a 60° rotation gives:

$$\frac{\sqrt{3}}{2}T$$

This distance places another 6-fold, which overlaps the first one, so no new 6-fold is created. The 6-fold has a subset of 3-fold, so additional 3-fold axes appear at the centroids of the equilateral triangles. Since 6-fold also has 2-fold as a subgroup, 2-fold axes appear along the diagonal and from 180° rotation followed by translation. Many symmetries emerge starting from just a 6-fold on a hexagonal cell.

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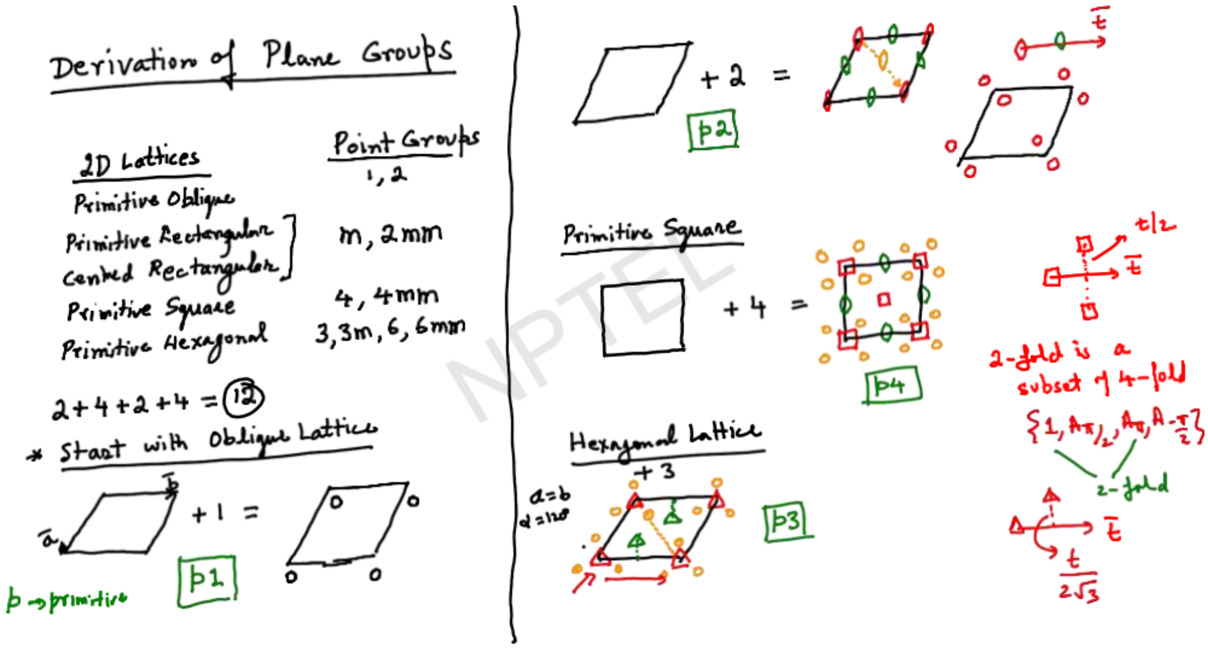

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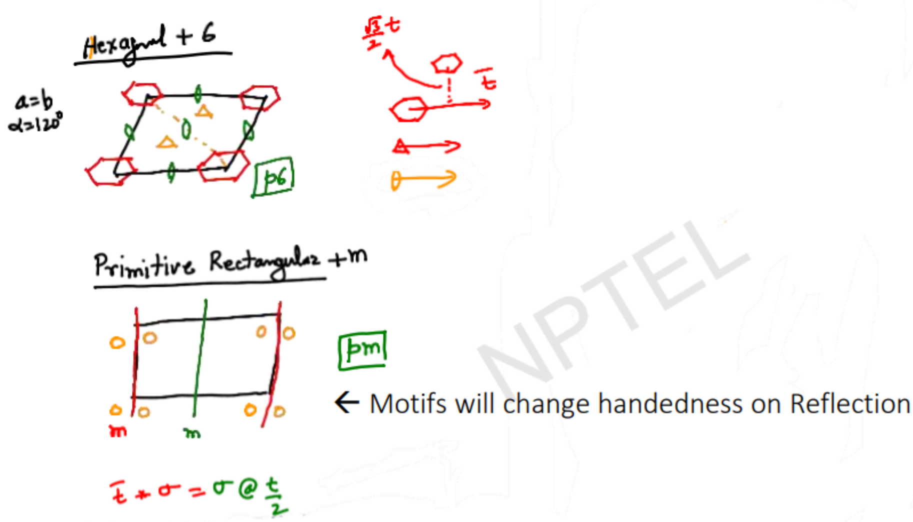

We have covered 1-fold, 2-fold, 3-fold, and 4-fold rotations. Reflection symmetry m has not been considered yet, nor higher point groups like $2mm$ or $4mm$.

Adding a mirror to a rectangular lattice (primitive or centered): Place a vertical mirror along the edge of the cell. Translation produces a mirror at the opposite edge. σ followed by a translation vector produces a mirror at the midpoint of the translation, giving a second mirror at $T/2$. Motifs can be placed, reflected across the mirrors, and propagated by translations to generate the full pattern.