CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES
Prof. Sandeep Sangal
IIT Kanpur
Lecture 21: Combining Translation with Point Symmetries-I

From this lecture onwards, we will start discussing plane groups. A plane group is basically a combination of a 2D lattice with a 2D point group. We have 5 2D lattices and 10-point groups, but not all point groups can be combined with any lattice. The compatibility is determined by the symmetry of that lattice.

The 2D lattices are:

- Primitive oblique

- Primitive rectangular

- Centered rectangular

- Primitive square

- Primitive hexagonal

These lattices are defined based on their required symmetries. For example:

- Primitive oblique can have a 1-fold or 2-fold rotational symmetry.

- Primitive rectangular must have at least a mirror symmetry.

- Centered rectangular also requires mirror symmetry.

- Primitive square requires a minimum 4-fold rotational symmetry.

- Primitive hexagonal can have a 3-fold or 6-fold rotational symmetry.

Based on this, the compatible point groups for each lattice are:

- Primitive oblique: point group 1 and 2

- Primitive rectangular and centered rectangular: point groups m and $2mm$

- Primitive square: point groups 4 and $4mm$

- Primitive hexagonal: point groups 3, $3m$, 6, and $6mm$

To see why compatibility matters, let's take an example with a square lattice. Draw some lattice points; a square lattice naturally has 4-fold rotational symmetry and multiple mirror planes. Now, place a motif on it. Suppose the motif consists of a larger atom with smaller atoms arranged symmetrically around it.

If this motif has a 4-fold rotational symmetry and mirrors, it corresponds to the point group $4mm$, which is compatible with the square lattice. Placing this motif at every lattice point preserves the lattice's symmetry and may even introduce additional symmetry, which is fine.

Now, consider a different motif on the same square lattice. Suppose the motif has a larger atom at the center and three smaller atoms arranged with 3-fold rotational symmetry and three mirrors, corresponding to point group $3m$. Placing this motif at every lattice point breaks the 4-fold rotational symmetry of the lattice.

Carefully examining the resulting pattern, you will see that the 4-fold rotation is gone. The 3-fold symmetry of the motif is also not preserved in the lattice pattern. The resulting symmetry is reduced to a 1-fold rotational symmetry with some mirror planes remaining.

In this case, we can no longer call the lattice a square lattice because it no longer has the required 4-fold rotational symmetry. This shows why only specific point groups are compatible with each lattice.

From the beginning of this course, we have been emphasizing that the lattice type is determined by the symmetry. For example, if a lattice requires a minimum symmetry of a mirror plane, it must be either a primitive rectangular or centered rectangular lattice.

This is not necessarily a centered cell. If we define a conventional unit cell, we could place it somewhere else, but here I am using a primitive cell with lattice points at the corners. Since it belongs to the rectangular crystal system, this is a primitive rectangular lattice. Even if the lattice parameters happen to satisfy $a = b$, this equality is coincidental; the lattice type is not defined by the parameter equality but by the

symmetry. This explains why only certain point groups are compatible with specific lattices.

With this in mind, we now look at how to develop plane groups. Before that, we need to understand how point symmetries combine with translation symmetry, because once we place motifs in a lattice, lattice translations come into play.

Let us revisit the previous question of two parallel mirrors spaced by a distance a. Let these be M_1 and M_2. We want to determine the symmetry operation resulting from the reflection σ_1 followed by the reflection σ_2.

Start with an asymmetric motif. Reflection by mirror M_1 maps this motif to motif 2 on the other side of the mirror, reversing handedness. Let motif 1 be at a distance δ from M_1. Then motif 2 is at the same distance on the other side. The distance from M_2 to motif 1 is $a - \delta$. Reflecting motif 2 by M_2, the distance on the other side will be $a + \delta$, producing motif 3, which becomes right-handed again.

Motif 1 reflected by M_2 would produce motif 4 at a distance $a - \delta$, left-handed.

So, from motif 1 to motif 3, the operation must preserve handedness. The only operation that does this is a translation along vector $\bar{t}$. The magnitude of this translation is

$$\bar{t} = (\delta + \delta) + (a - \delta) + (a + \delta) = 2a$$

Thus, the symmetry operation resulting from σ_1 followed by σ_2 is a translation with magnitude $2a$.

Notice that a mirror plane will also appear, essentially being translated along with this translation. Conversely, if we start with a mirror and a translation t, the translation moves the mirror along the lattice, producing a reflection plane at $a/2$, which we can denote as m'.

It is also possible to combine a translation with a mirror where the translation is at an angle to the mirrors normal. This creates another type of symmetry operation. These translations are lattice translations.

We will not solve this angled translation case yet, but it leads to a symmetry operation called a glide, which will be discussed in a later lecture.

This brings us to the end of the lecture. In the next lecture, we will develop a translation matrix, similar to rotation and reflection matrices, which will allow us to combine translations with other point symmetries using matrix multiplication to obtain new operations.

(Refer Slide Time: 21:27)