CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 13: 2D Crystal Systems and Lattices - II

In the previous lecture, three two–dimensional crystal systems were developed using the point symmetries 1, 2, 3, 4 and 6; the mirror symmetry remained unused. Continuing from that point, a mirror symmetry is now added to the translation vector $\overline{a}$, that is, reflection symmetry is introduced.

Let $\overline{a}$ be a translation vector and let a mirror, denoted m, be placed perpendicular to $\overline{a}$. The question arises as to where the second vector $\overline{b}$ may be placed. If $\overline{b}$ is chosen in an arbitrary orientation, the mirror will reflect $\overline{b}$ into a different orientation, denoted $\overline{b'}$. Suppose lattice points exist at the ends of these vectors. The lattice spacing along $\overline{a}$ (for example between lattice points 1 and 2) has some value a.

The spacing between the corresponding lattice points 3 and 4 along the reflected direction would then, in general, be different because $\overline{b}$ was arbitrary, and the lattice translation condition would be violated. Therefore, the arbitrary orientation for $\overline{b}$ is not acceptable if translation symmetry is to be preserved.

One way to satisfy translation symmetry is to place $\overline{b}$ along the mirror itself. In that configuration no inconsistency arises. The unit cell can then be chosen as a rectangle with lattice points at the corners and the translation vectors $\overline{a}$ and $\overline{b}$ orthogonal to each other. This yields a primitive rectangular unit cell, often described as a rectangular crystal system in which a need not equal b and the angle between the vectors is 90° ($a \neq b$, $\alpha = 90°$)

An alternative configuration is obtained by changing the orientation of a while keeping the mirror horizontal. Under reflection, the vector $\overline{a}$ is mapped to a vector $\overline{b}$ on the other

side of the mirror. If a unit cell is constructed from these vectors, the resulting primitive cell is a rhombus (diamond shaped), and the lattice points occupy the corners of that rhombus. Drawing adjacent rhombus cells and populating all corners with lattice points produces a valid lattice.

An alternative conventional cell for the same lattice can be chosen which is rectangular: in that alternative cell there are lattice points at the four corners and one lattice point at the center of the rectangle. The vectors in this conventional cell are orthogonal and the angle is 90°, while the side lengths need not be equal. This conventional cell is therefore a centered rectangular unit cell (also called a centered rectangle), which is non-primitive and contains two lattice points per cell, one from the corners and one from the centre.

Thus, although one geometric representation of the lattice is a rhombus (primitive), the conventional choice may be a centered rectangle. In the rhombus the constraint is that all sides are equal ($a = b$), while in the centered rectangle the constraint is that the angles are 90° (with a not necessarily equal to b).

In both cases there is at least one constraint on the unit cell parameters, and both representations fall under the rectangular crystal system. Accordingly, analogous to the cubic Bravais lattice family (simple, body-centered, face-centered), the two-dimensional rectangular system admits both primitive rectangular and centered rectangular conventional cells. The essential defining symmetry for the rectangular crystal system is the presence of a reflection symmetry.

In conclusion, the two-dimensional crystal systems developed are four in number: oblique, rectangular, square, and hexagonal. These give rise to five distinct two-dimensional lattices when conventional unit cells are counted; the common conventional primitive cells are primitive oblique, primitive rectangular, and primitive square. The centered rectangular (conventional) cell provides an additional conventional representation for the rectangular system.

From the four two–dimensional crystal systems, oblique, rectangular, square and hexagonal. The corresponding lattices include the primitive cases for oblique, rectangular, square and hexagonal, with the second rectangular unit cell added as the centered rectangular lattice. This yields a total of five two–dimensional lattices. In contrast, three dimensions contain fourteen lattices distributed across seven crystal systems, whereas two dimensions contain four crystal systems and the five corresponding Bravais lattices.

To understand the relation between lattice symmetry and crystal symmetry, consider the primitive rectangular lattice. This lattice may be described by a primitive rectangular cell with lattice points at the corners. The symmetry elements of the lattice can be located directly on the lattice itself. Because reflection symmetry was the defining feature of the rectangular lattice, mirror lines must necessarily exist.

These mirrors pass through columns of lattice points and also occur midway between such columns. When the primitive rectangular unit cell is isolated, its repetition generates both the full lattice and all symmetries present in the lattice. Additional symmetries appear as well: twofold rotational symmetry exists at each lattice point, at the midpoints of cell edges and at the center of the unit cell. These twofold rotation centers can also be drawn at corresponding positions throughout the lattice.

To examine the effect of adding a motif, redraw the lattice, select a unit cell and place at each lattice point a motif possessing only reflection symmetry. A convenient choice is an asymmetric pair reflected about a single mirror: the combined motif has exactly one mirror symmetry. Adding this motif to every lattice point by translation creates the overall crystal pattern.

On inspecting the resulting pattern, the original horizontal mirrors of the lattice are absent; no horizontal reflection plane remains. Vertical mirrors, however, do survive. These vertical mirrors pass through the lattice points and also lie between adjacent

columns of lattice points, reflecting the motifs accordingly. The twofold rotational symmetries that existed in the lattice are also lost in the crystal pattern.

Thus, the final crystal pattern possesses neither horizontal mirrors nor twofold rotational symmetries; only the vertical mirrors remain. This demonstrates a fundamental principle: the symmetry of a crystal is always less than or equal to the symmetry of the underlying lattice. A pure lattice possesses the maximum possible symmetry allowed by its crystal system. When a motif is placed on the lattice to form the crystal, the resulting crystal symmetry may reduce depending on the symmetry of the motif.

Nevertheless, the crystal must retain at least the minimum symmetry required for classification within its crystal system. In the present example, the final pattern still contains a single set of reflection symmetries and is therefore still classified as belonging to the rectangular crystal system.

This principle will reappear in later discussions, particularly in the study of point groups, space groups and the general notion of groups, which will be taken up in the next lecture.

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