CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

Prof. Sandeep Sangal
IIT Kanpur

Lecture 10: Translation and Point Symmetries

In the last few lectures, we have introduced the basic elements of crystallography, in which lattice, motif, crystals, directions and planes, Miller indices, and related concepts were discussed. One of the key points emphasized was that all lattices and crystals possess translation symmetry. To reiterate this before moving into other symmetry elements of a lattice and a crystal, translation symmetry is a definitive requirement for any lattice.

Here we have a set of lattice points arranged in an orderly manner that exhibits translation symmetry. Translation symmetry means that if a translation vector is applied to shift all lattice points, the lattice must coincide with itself. For example, a translation vector is drawn, and upon shifting the lattice points by this vector, the lattice indeed comes into self-coincidence, confirming that this is legitimately a lattice. This is not the only such vector; there are other lattice vectors as well.

For instance, another vector joining one lattice point to another is also a lattice vector, and shifting the entire infinite lattice along this vector again results in every lattice point coinciding with another lattice point (Look at the images attached below). Translation symmetry is therefore a fundamental symmetry of a lattice.

However, a lattice as well as a crystal possesses many additional symmetry elements, and these are the ones I now introduce. Consider a lattice similar to the previous one. Suppose I begin looking for other symmetries. Translation symmetry has already been established, but now let us examine additional possibilities. If I draw a line through a column of lattice points, this line acts as a mirror because it reflects lattice points from right to left and left to right across the entire lattice. After the reflection operation, the lattice again comes into self-coincidence, just as it does under translation. This is one mirror line, or in three dimensions, a mirror plane. In two dimensions, it remains a mirror line.

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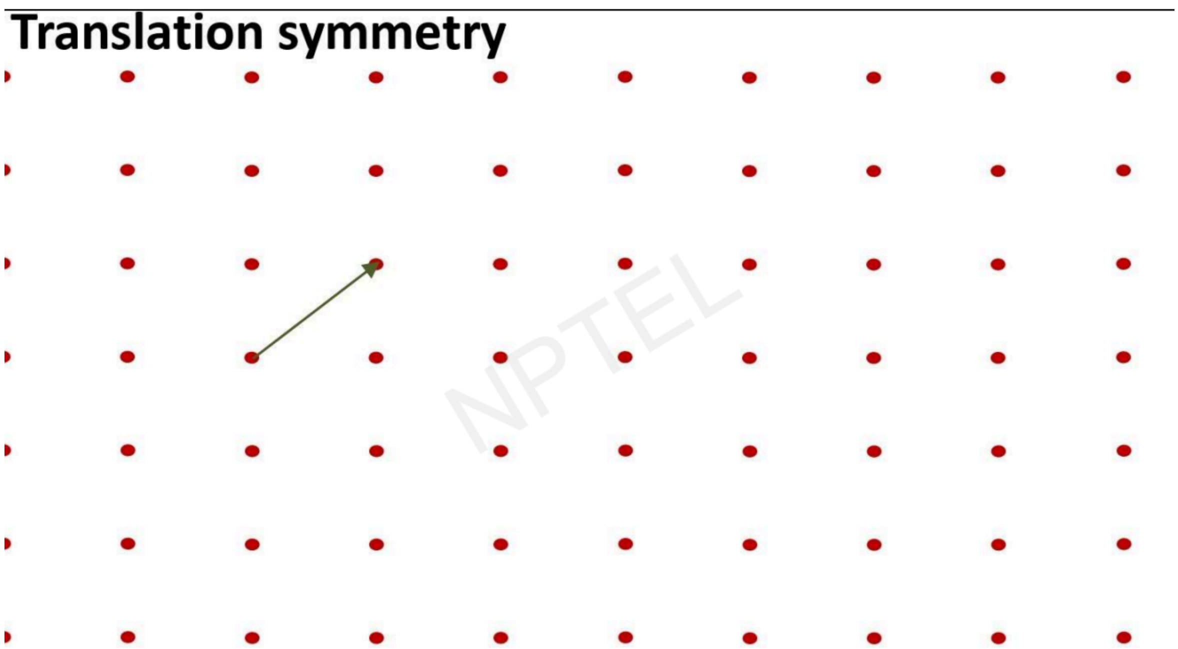

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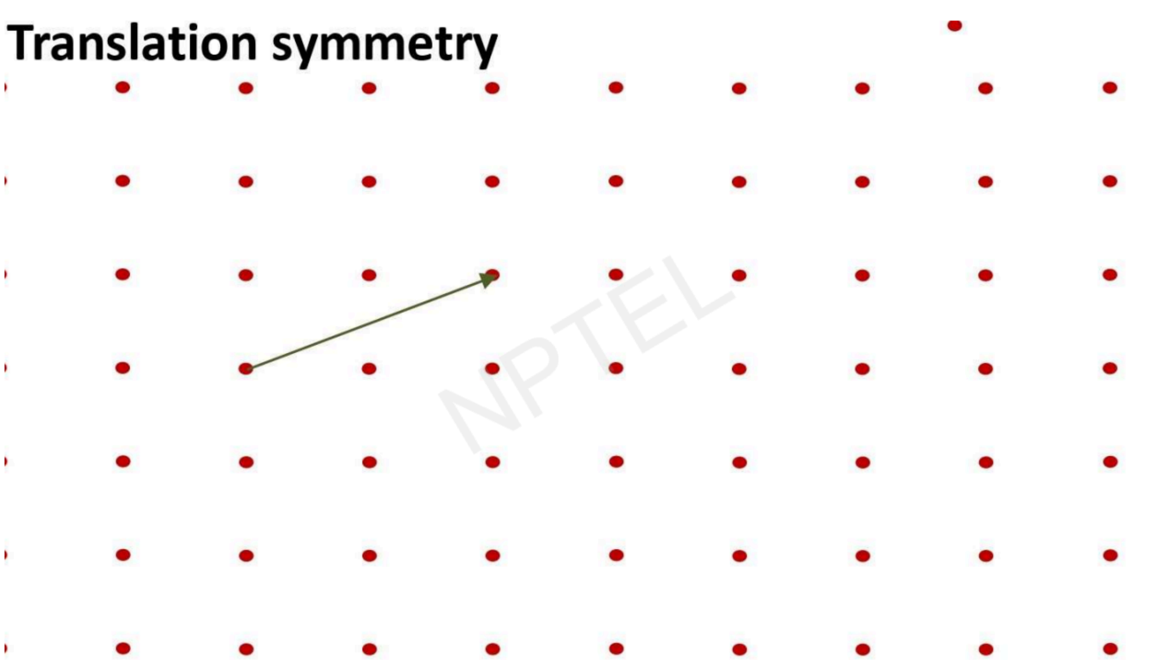

There are mirror lines along every column of lattice points, and the translation symmetry would also translate the mirrors along with the lattice points. However, these are not the only mirrors present. There exist additional mirrors located between the columns of lattice points. This third mirror similarly reflects lattice points on either side into positions of coincidence. These are not the only reflection symmetries; one can also identify horizontal mirrors. These horizontal mirrors extend across the entire lattice space. Although only a few are drawn, every horizontal row of lattice points has a mirror, and between each pair of horizontal rows, additional mirror lines appear.

If we examine the pattern carefully, more mirror lines can be identified. One may pause and think about this: taking four lattice points at the corners of a square, additional mirrors can be drawn along the diagonals. These diagonal mirror lines also extend across the lattice and reflect lattice points into self-coincidence. These diagonal mirrors can similarly be drawn throughout the lattice.

Now, let us consider whether further symmetries exist. At the intersection of several mirrors, a square is formed. If this square is rotated about an axis normal to the page through a certain angle, the lattice points again come into self-coincidence. For instance, consider a small square drawn to indicate a rotation point or rotation axis. A rotation of 90° brings the lattice into self-coincidence, and repeated 90° rotations about this axis continuously reproduce the same lattice. These are not the only rotational symmetries present. Every lattice point serves as a center of 90° rotation, known as four-fold rotational symmetry.

There is yet another fourfold symmetry located at the center of a square formed by four surrounding lattice points. Although no lattice point lies exactly at this position, rotating the lattice by 90° about this point again results in self-coincidence.

Even this does not exhaust all the rotational symmetries. If one examines the centers of the edges formed by intersections of mirror lines, another type of rotational symmetry appears, distinct from the previous ones because it requires a different angle of rotation rather than the 90° one used earlier. Here, one would need to rotate by 180° to bring the lattice into self-coincidence, and because of the symmetry of the entire lattice, one finds additional centers exhibiting the same 180° rotational behavior. These are referred to as twofold rotational symmetries, and I will explain this terminology shortly. All the centers located between the two four-fold rotation centers also possess this two-fold rotational symmetry. With this, the rotational symmetries and the mirror planes present in this particular lattice are complete.

I now turn to the question of how this lattice should be classified. If we consider a two-dimensional crystal system, what should this be called? To approach this, let us examine possible unit cells. Although an infinite number of unit cells may be chosen, one example is a cell in which the axes a and b meet at 90° and the magnitudes of a and b are equal. Although this appears rectangular in the drawing, the lattice points actually lie at the corners of a square. Another possible choice of unit cell may have $a \neq b$ and the angle between them not equal to 90°. The point here is that one may choose any convenient unit cell, but the symmetries remain unchanged.

Therefore, the crystal system to which the lattice belongs must be determined based on symmetry and not on the specific unit cell chosen, as mentioned earlier. In two dimensions, if a lattice possesses four-fold symmetry, it is classified as a square crystal system regardless of the chosen unit cell. The natural choice for the unit cell in a square crystal system is the primitive square cell in which $a = b$ and the angle between the axes is 90°. This is the most direct representation, yet if one chooses the second unit cell or any other unconventional cell, that remains acceptable. The lattice continues to belong to the square crystal system because it must possess at least one fourfold rotational symmetry, corresponding to a 90° rotation.

Now consider the second unit cell where $a \neq b$ and the angle is not 90°. Even here constraints exist. In the square cell, the constraint $a = b$ arises from the presence of 90° rotational symmetry. In the second unit cell, although written as $a \neq b$, there remains a relationship between them because the a-axis corresponds to the diagonal of the square primitive cell. Thus, there is a constraint relating a and b, and this relationship is clearly $a/b = \sqrt{2}$. This constraint also follows from the underlying rotational symmetry. Consequently, this lattice is classified as a square crystal system regardless of the chosen unit cell. Even for other arbitrary unit cells, constraints on a, b, and the angle persist. In fact, the angle shown as not 90° is actually 45°, corresponding to the angle made by the diagonal of a square with its edges.

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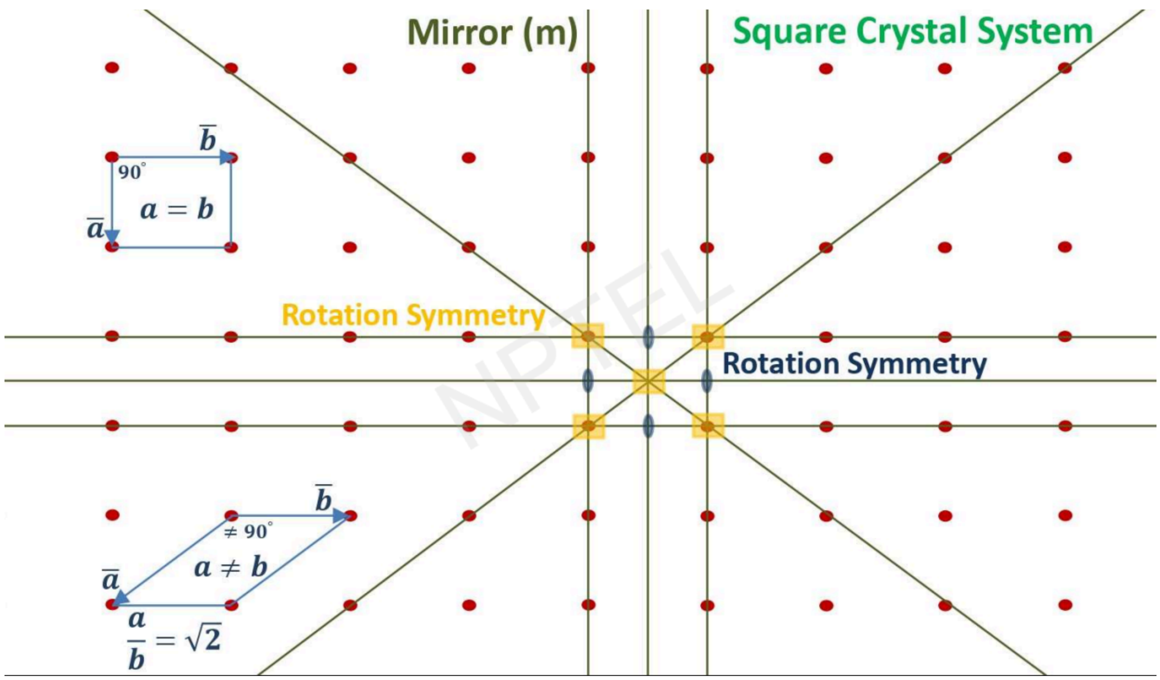

With this clarification, it should be clear that crystal systems are determined by the symmetries present in the lattice. Let us now move into a more detailed discussion of these symmetries, such as rotation and reflection, and later see that additional types also exist. The first essential point is that unit cells, lattices, and crystals have translation symmetry, which must be present for any arrangement to be considered a lattice of points.

I now introduce point symmetries. Under point symmetries we have rotational symmetry, and I will explain the origin of the term "point" shortly. Rotation symmetry exists in two dimensions as well as three dimensions, but it does not exist in one dimension. Earlier I used the expression "n-fold" or "four-fold" rotational symmetry, which I now generalize. In the example of a 90° rotation, I referred to it as a fourfold symmetry. If one rotates an object four times by 90°, it returns to its original orientation, since $4 \times 90^{\circ} = 360^{\circ}$.

Thus, an n-fold rotational symmetry means that the minimum rotation angle required to bring an object into self-coincidence is given by $\theta = \frac{2\pi}{n}$, where n is an integer. The values of n can be $1, 2, 3, 4, 5, ...$ For example, when I say fourfold symmetry, $n = 4$, and the minimum rotation angle is $\theta = \frac{2\pi}{4} = \frac{\pi}{2}$. Thus, fourfold symmetry corresponds to a minimum rotation of $\pi/2$, or 90°. If we examine the case $n = 1$, then $\theta = \frac{2\pi}{1}$, means a full 360° rotation. Now all objects possess one-fold rotational symmetry because they return to self-coincidence after a rotation of 360° about any axis or point, and therefore onefold symmetry is also regarded as no symmetry.

Any n-fold rotational symmetry axis consists of a set of individual operations, and it is useful to examine them through examples. For a twofold symmetry, $\alpha = \frac{2\pi}{2} = \pi$, and one operation is a rotation of 180°, while another operation is a rotation of 2π, which is the full 360° rotation. Thus, the set of individual operations consists of $\{\pi, 1\}$, where 1 denotes the identity operation, sometimes also written as E. The identity corresponds to 2π, and this holds for all objects irrespective of their rotational symmetries.

For a threefold symmetry, $\alpha = \frac{2\pi}{3}$, which corresponds to a rotation of 120°. The individual operations are $\frac{2\pi}{3}$, then another $\frac{2\pi}{3}$ giving $\frac{4\pi}{3}$ or 240°, and a further 120° results in 2π, which is again written as the identity 1. For a fourfold symmetry, $\alpha = \frac{2\pi}{4} = \frac{\pi}{2}$ or 90°. The allowed operations are $\frac{\pi}{2}$, then another $\frac{\pi}{2}$ giving π or 180°, then $\frac{3\pi}{2}$ or 270°, and finally the identity 1.

For a fivefold symmetry, $\alpha = \frac{2\pi}{5}$, which is 72°, and one may similarly write $\frac{2\pi}{5}$ and four additional operations obtained through repeated additions of the same angle. In general, one can write the full set of operations for any n-fold rotation. In principle, n can be any natural number, although restrictions on possible values of n will arise later. These point symmetries apply to both two and three dimensions.

Next, consider reflection symmetry, which involves mirror lines or mirror planes and occurs in one, two, and three dimensions. The symbol m is typically used to denote a mirror plane, while σ represents the reflection operation. The set of individual operations for reflection is $\{\sigma, 1\}$, consisting of the reflection itself and the identity.

Now consider inversion symmetry, which occurs in three dimensions but not meaningfully in one or two dimensions, although two dimensions possess a related but distinct concept that we do not use here. Inversion symmetry is defined through an inversion center. Suppose we have a coordinate system and a point located at some position P a distance p from the origin. Extending the axes, if we connect the point P to the origin and continue the line an equal distance beyond the origin, we reach a second point Q. The origin then functions as the inversion center. This inversion operation changes the handedness of objects, meaning a right-handed object becomes left-handed after inversion. The same reversal of handedness also occurs in reflection symmetry, and we will examine this in greater detail later.

There is also improper rotation, which is another class of rotational symmetry. The terminology used for this includes rotoinversion or roto-reflection, although our preferred term is rotoinversion. This symmetry also involves a change in handedness and occurs in three dimensions.

Before concluding, it is necessary to discuss coordinate changes resulting from symmetry operations. In the case of reflection, if the coordinates of a point are (x, y, z), one coordinate changes sign while the others remain the same, for example $(\bar{x}, y, z)$, where the plane yz serves as the mirror plane. In rotation, two coordinates change sign; for instance, x becomes $\bar{x}$, y becomes $\bar{y}$, and z, being the rotation axis, remains unchanged. In inversion, all three coordinates change sign, so if a point P has coordinates (x, y, z), the inverted point Q has coordinates $(\bar{x}, \bar{y}, \bar{z})$.

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