B.Sc. Fourth Year

Reference Book:
Kittel, C., Introduction to Solid State Physics, 8^{th} ed., John Wiley & Sons Ltd, India (2005)

Symmetry Operations

A *symmetry operation* is that which transforms the crystal to itself, i.e., a crystal remains invariant under a symmetry operation. These operations are translation, rotation, reflection, and inversion. The translation operation applies to lattice only while all thre remaining operations and their combinations apply to all objects and are collectively know as point symmetry operations. The inversion operation is application only to three dimensional crystals.

Translation The translation symmetry follows from the orderly arrangement of a lattice. It means that a lattice point $\vec{r}$, under lattice translation vector operator $\vec{T}$, gives another point $\vec{r'}$ which is exactly identical to $\vec{r}$, i.e.,

$$\vec{r'} = \vec{r} + \vec{T}$$

Rotations A lattice is said to possess the rotation symmetry if its rotation by an angle θ about an axis transforms the lattice to itself. Also, since the lattice always remains invariant by a rotation of 2π, the angle 2π must be an integral multiple of θ, i.e.,

$$n\theta = 2\pi$$

The factor n takes integral values and is known as multiplicity of rotation axis. The possible values of n which are compatible with the symmetry requirement are 1,2,3,4, and 6. A rotation corresponding to the value of n is called $n - fold$ rotation. For example, a two dimensional square lattice has 4-fold rotational symmetry.

Reflection A lattice is said to possess reflection symmetry if there exists a plane in the lattice which divides it into two identical halves which are mirror images of each other.

All the above symmetry operations are applicable to a two dimensional lattice.

Inversion Inversion is a pint operation which is applicable to three dimensional lattice only. The symmetry element implies that each point located at $\vec{r}$ relative to a lattice point has an identical point located at $-\vec{r}$ relative to the same lattice point.

- Symmetry operations like translation and rotation leave motif unchanged, whereas reflection or inversion changes the character of the motif from right handed to left handed and vice-versa.
- A translation repeats the motif an infinite number of times in a given direction whereas the other operations replear the motif a finite number of times.
- **Point operation:** The translation operation applies to lattice only whle the remaining operation and their combinations apply to all objects and are collectively known as point symmetry operations .

Consider a row of lattice points A, B, C, and D as shown in figure. Let T be the lattice translation vector and let the lattice have n-fold rotational symmetry with rotaion axes passing throung the lattice points perpendicular to the planne of paper. Rotation by an angle θ about ponts B and C in the clockwise and anticlockwise directions respectively yield points B' and C' which must be identical to B and C. Thus the ponts B' and C' must also be lattice points and should follow lattice translation symmetry. Hence B' C' must be some integral multiple of BC, i.e.,

$$B'C' = m(BC)$$

$$2T\cos\theta + T = mT$$

$$\cos\theta = (m-1)/2$$

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Figure 1: Geometry used to prove that only 1, 2, 3, 4, and 6 -fold rotation axes are permissible

where m is an integer. Since $|\cos\theta| \leq 1$, the allowed values of m are 3, 2, 1, 0 and -1. These correspond to the allowed values of θ as $0°$ or $360°$, $60°$, $90°$, $120°$, and $180°$ respectively. Hence from equation

$$n\theta = 2\pi,$$

the permissible values of n are 1, 6, 4, 3, and 2. Thus we conclude that 5-fold rotation is not permissible because it is not compatible with the lattice translation symmetry. Similary, other rotations, such as 7-fod rotation are also not permissible.