Crystal Structure

The Law of Symmetry:

The law of symmetry states that all crystals of the same substance has the same elements of symmetry. Symmetry is an unique regularity observed among the atoms or ions of the crystal from various aspects due to their particular type of ordered arrangement. Symmetry operation is an at which when done on a crystal the crystal attains a state which is the mirror image or replica of the initial state of the crystal. A crystal is said to have a plane of symmetry when it is divided by an imaginary plane into two halves such that one half is the mirror image of the other half.

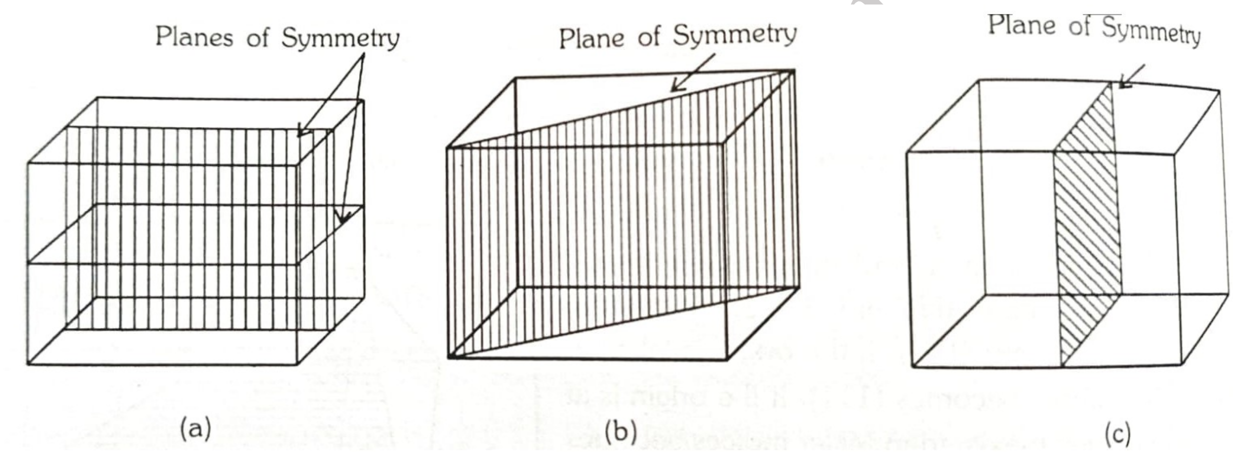

Fig 13:Planes of symmetry of a cube from different direction.

A line of symmetry is an imaginary line drawn through the centre of the crystal such that when crystal is revloved about that axis through an angle of 360° the crystal attains n-times its original stat and the axis is then called n-fold axis of symmetry. The value of n may be 2.3.4.6 but it cannot be 5. i.e. a five-fold axis of symmetry is absent in a crystal. For n-fold axis of symmetry the crystal attains its own state for every 360°/n rotation of crystal about the axis. Thus for a two -fold axis of symmetry a minimum rotation by 180° brings the crystal to its initial state.

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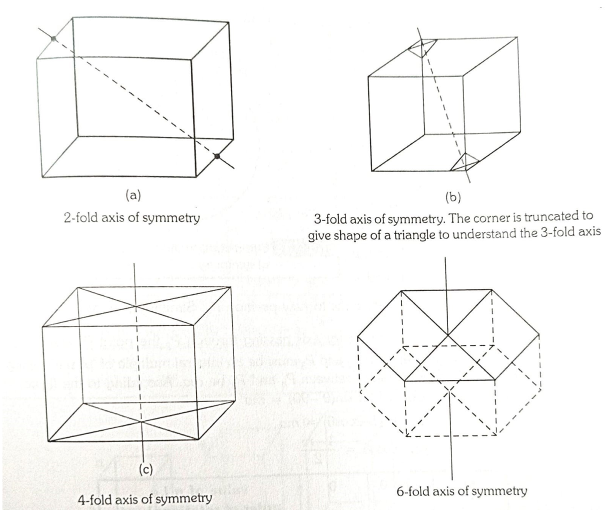

Fig14: Different axis of symmetry

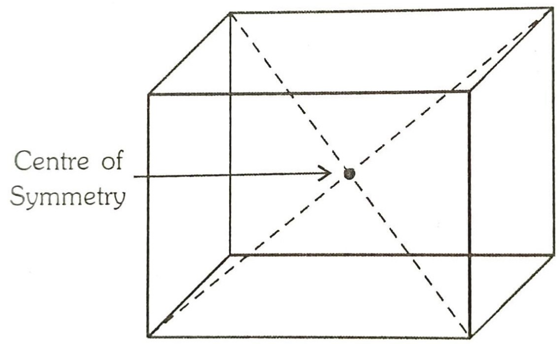

Fig15: Centre of symmetry

A crystal has a centre of symmetry when every atom of a face has its replica when the atom is connected to the centre of symmetry by a line and the line is extended to the same distance. A crystal have only one centre of symmetry. The total number of line, plane and centre of symmetry is called elements of symmetry. A cube has 23 elements of symmetry of which three four-fold, four three-fold. six two-fold axis of symmetry, nine planes of symmetry and one centre of symmetry. In a perfecty developed crystal only, all the symmetry elements have their significance.

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Absence of five-fold axis of symmetry:

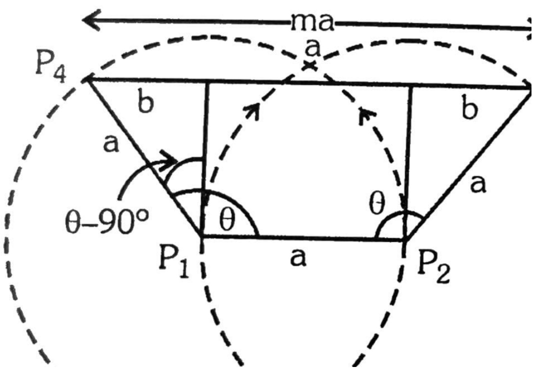

Fig.16: Symmetry operation showing absence of five fold axis of symmetry

Whenever a crystal possesses n-fold rotational axis then on rotation of the unit crystal through the symmetry axis by 360°/n old lattice points take new arrangement such that the new arrangement of lattice points can't be distinguished from the old arrangement. During such a rotation translational symmetry of the crystal is maintained. ie. if along x-coordinate in the old arrangement primitive translation i.e. the minimum separation between two same adjacent atoms or ions be 'a' then in the new arrangement the gap between two same atoms or ions must be 'a' or an integral multiple of 'a' say ma. Let us carry out such a rotation anticlockwise by $\theta = (360^o)/n$ so long the symmetry axis passing through the lattice point P_1. During rotation point the P_2 shifts to new position P_4. Similarly if rotation by is carried out clockwise along the symmetry axis passing through P_2 the point P_1 takes the new position P_3. Therefore the gap between P_4 and P_3 must be an integral multiple of 'a' maintaining the translational symmetry. Let the distance between P_4 and P_3 be ma. According to the figure $a + 2b = ma$ or, $a + 2a \sin(\theta - 90) = ma$

or, $a(1 - 2\cos\theta) = ma$ or, $\cos\theta = (1 - m)/2$

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m	cos θ	θ	value of n i.e. order of rotational axis
0	$\frac{1}{2}$	60°	$\frac{360°}{60°} = 6$
1	0	90°	$\frac{360°}{90°} = 4$
2	$-\frac{1}{2}$	120°	$\frac{360°}{120°} = 3$
3	−1	180°	$\frac{360°}{180°} = 2$

More higher values of m is not possible since value of cos 0 can't be greater than 1. So five-fold rotational axis is absent in crystal.