Symmetry Operations

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What is Symmetry Operation?

An operation that takes the crystal into itself is called a symmetry operation.
i.e. when a symmetry operation is performed on lattice, it leaves the lattice invariant.

Types of Symmetry Elements

- ✓Pure Translation: T= $n_1\mathbf{a}+n_2\mathbf{b}+n_3\mathbf{c}$
- ✓Proper Rotation: through an angle ϕ
- ✓Reflection: across a line in 2D and across a plane in 3D
- ✓Inversion through a point
- ✓Improper rotation: Rotoreflection/rotoinversion

Translation

- Translation symmetry means that the environment about a point in the lattice remains unchanged when translated by lattice translation vector $T= n_1\mathbf{a}+n_2\mathbf{b}+n_3\mathbf{c}$

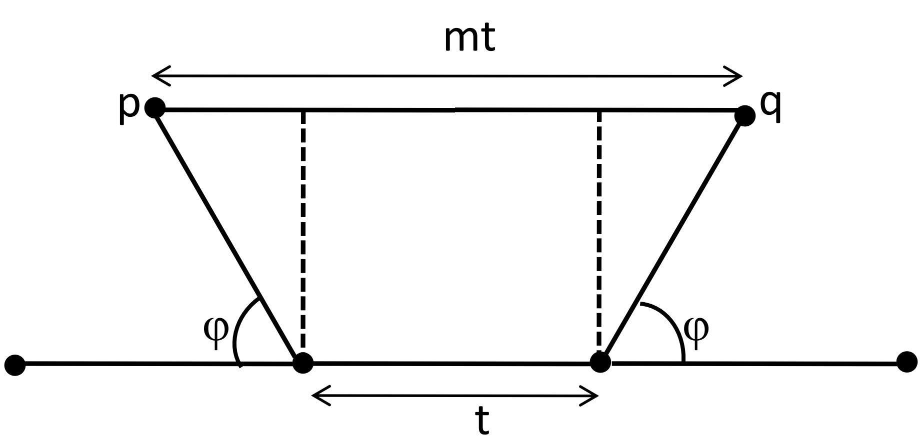
Proper Rotation

- If the lattice is invariant under rotation about an axis through an angle $\varphi=2\pi/n$, the axis is said to have n-fold symmetry.
- The rotational symmetries allowed are only 1, 2, 3, 4 and 6 fold.

Allowed n fold rotations

- Consider 1 dimensional lattice with translation vector t.
- Consider two rotations of angle φ producing 2 lattice points, p and q. The separation between p and q must be in integral multiples of t say mt depending on φ.
- By construction
- $mt = t + 2t\cos\varphi$ or $m-1 = 2\cos\varphi$, let $m-1=N$ an integer
- $N = 2\cos\varphi$ or $\cos\varphi = N/2$ where $N=0,\pm1,\pm2,\ldots$
- Since cosφ lies between ±1, the various values of N,φ,n can be found

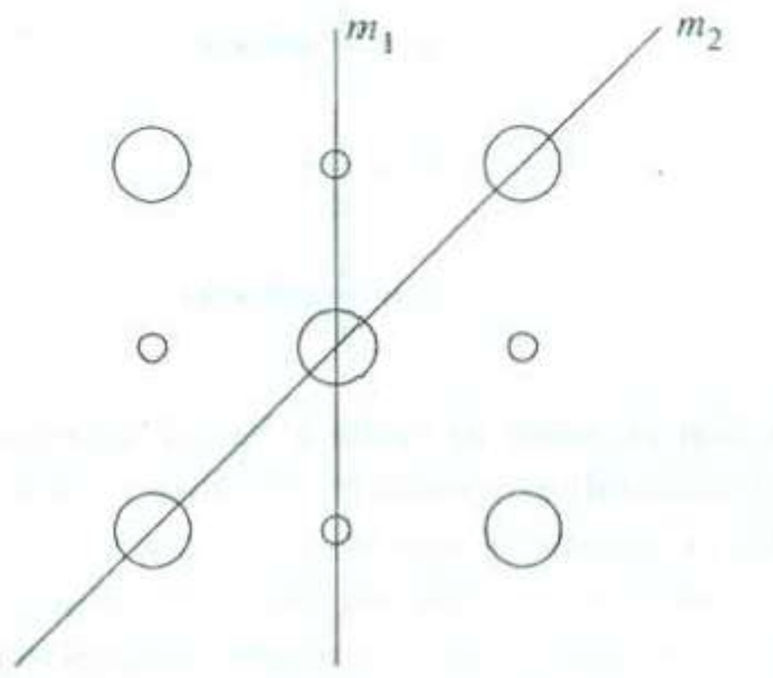
N	cosφ	φ	n
-2	-1	180	2
-1	- ½	120	3
0	0	90	4
1	½	60	6
2	1	360/0	1



Mirror Reflection

In this operation the reflection of a structure at a mirror plane passing through a lattice point leaves the lattice invariant. The mirror plane is composed of the atoms lying on the concerned imaginary plane. The mirror plane is symbolically represented by ‘m’.

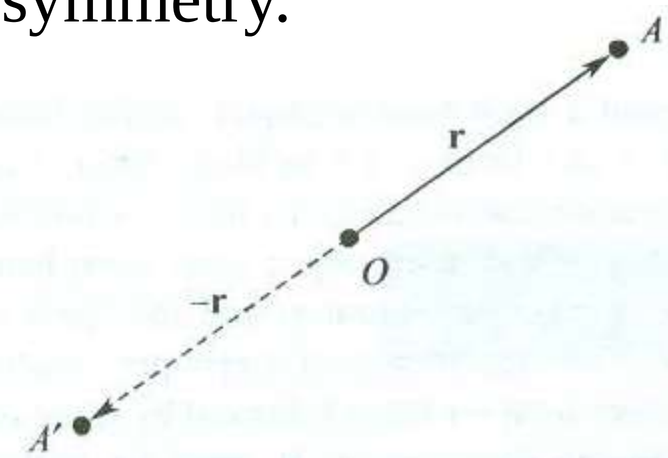
A lattice cut along the mirror plane and placed in front of the mirror, the image completes the other half of the lattice.



Inversion

Let the position vector of a lattice point be r, and origin be some other lattice point. If to every lattice point at **r** there is another lattice point at position vector –**r**, we say that the lattice has inversion symmetry. The origin is said to be the centre of inversion symmetry, symbolically represented by ‘$\overline{i}$’.

Every Bravais lattice has inversion symmetry.



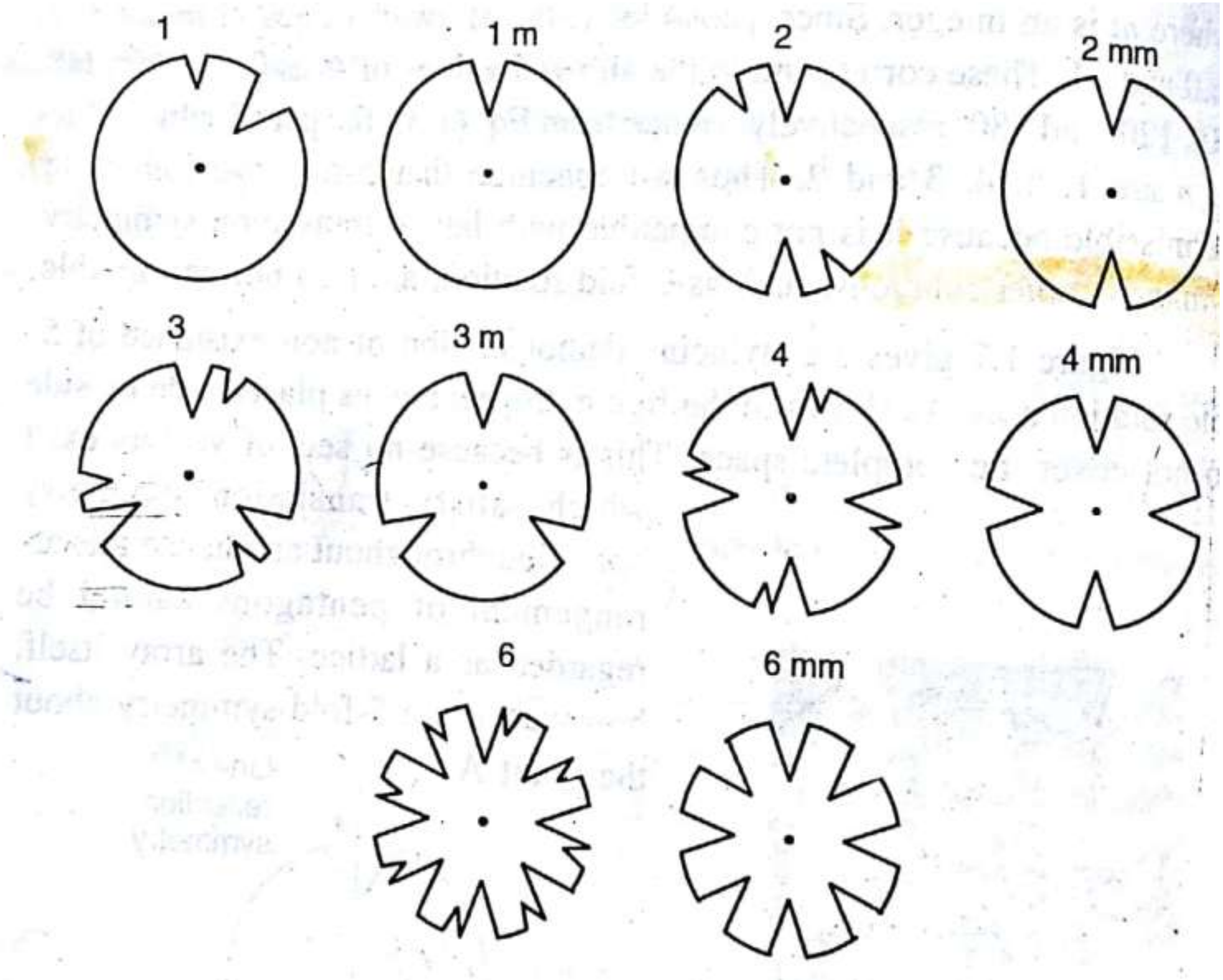
Improper Rotation

- **Rotoreflection:** If a rotation and a reflection is combined to form a single hybrid operation, the resulting operation is called rotoreflection. It is represented by a tilde over the numerical symbol corresponding to rotation axis, e.g. $\tilde{1}$,$\tilde{2}$ etc.
- **Rotoinversion:** If rotation is combined with inversion it produces rotoinversion. It is represented by placing a bar over the numerical symbol corresponding to rotation axis, e.g. $\overline{1}$, $\overline{2}$, etc.

Point Groups

- Groups formed by combination of rotation, reflection and inversion symmetry operations about a fixed point forms a point group.
- In this symmetry operations at least one point remains at rest.
- In 2 dimensions the combination of rotation and reflection yield 10 different point groups designated as 1, 1m, 2, 2mm, 3, 3m, 4, 4mm, 6, 6mm
- In 3 dimesions addition of inversion leads to a total of 32 point groups.

10 two dimensional Point groups



Space Groups

- The group of all symmetry elements of a crystal structure is called a space group.
- Space groups are combinations of translational symmetry of unit cell and symmetry operations such as rotation , reflection, rotreflection, rotoinversion, screw translation and glide reflection symmetry operations.
- It determines the symmetry of crystal structure as a whole. There are 17 and 230 distinct space groups in two and three dimensions respectively.