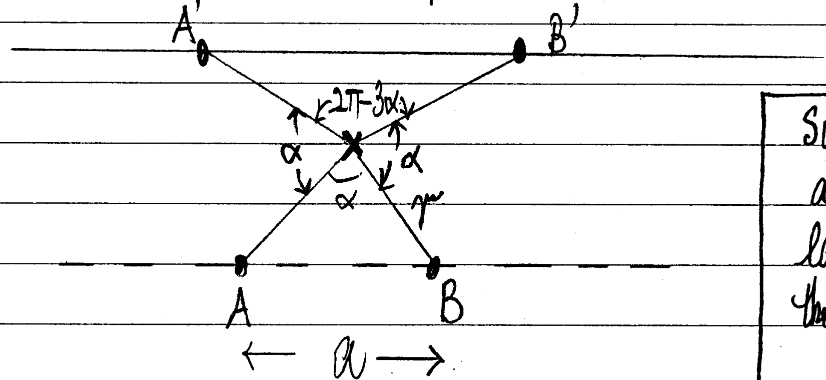
Appendix A

- This appendix gives an argument on why only 2, 3, 4, 6-fold symmetry axes are observed in crystals.

Consider a 2D (easier to visualize in 2D) lattice (but the argument also holds in 3D). Let **x** be a point in space (it doesn't have to be on a lattice point).

We suppose the lattice remains unchanged by a rotation of angle α through an axis passing through point **x**.

Consider a lattice point A. After rotation, it is at B.



Since the lattice is unchanged after rotation, there must be a lattice pt. original at B gets to the pt. B', and a pt. A' that moves into A.

Suppose there are no lattice pts closer to x than A and B

Let $AB = a$

- Consider the line joining AB. The line passes through infinitely many lattice points with a separation a.

Since we have a lattice, any line parallel to the one joining A and B must also pass through lattice points with separation a.

See Figure: B' is obtained by rotating anticlockwise by α (from B).
A' is obtained by rotating clockwise by α (from A).

$A'B' \parallel AB$ AND A' and B' must be locations of lattice pts.

$\therefore$ Separation between A' and B' $= na$, where $n =$ integer

In addition, A, B, A', B' are all points on a circle with x being the center.

$\therefore$ AB and A'B' are chords on a circle.

Let $r =$ radius of circle (see figure)

$$AB = 2r\sin\left(\frac{\alpha}{2}\right) \quad ; \quad A'B' = 2r\sin\left(\frac{3\alpha}{2}\right)$$

But $$\frac{A'B'}{AB} = n = \frac{\sin\left(\frac{3\alpha}{2}\right)}{\sin\left(\frac{\alpha}{2}\right)} = \frac{3\sin\left(\frac{\alpha}{2}\right) - 4\sin^3\left(\frac{\alpha}{2}\right)}{\sin\left(\frac{\alpha}{2}\right)}$$

Solve for $\sin\left(\frac{\alpha}{2}\right)$:

$$\sin^2\left(\frac{\alpha}{2}\right) = \frac{3-n}{4}$$

But $0 \leq \sin^2\left(\frac{\alpha}{2}\right) \leq 1$, so n can only take on the values

$-1, 0, 1, 2, 3$

For $n = -1$, $\alpha = \pm\pi$ [2-fold]

For $n = 0$, $\alpha = \pm\frac{2\pi}{3}$ [3-fold]

For $n = 1$, $\alpha = \pm\frac{\pi}{2}$ [4-fold]

For $n = 2$, $\alpha = \pm\frac{\pi}{3}$ [6-fold]

For $n = 3$, $\alpha = 0$ or 2π [trivial]

$\boxed{\therefore \text{ Only 2, 3, 4, 6-fold rotational axes can occur in crystals.}}$

In particular, we don't expect 5-fold rotational axes in a crystal.