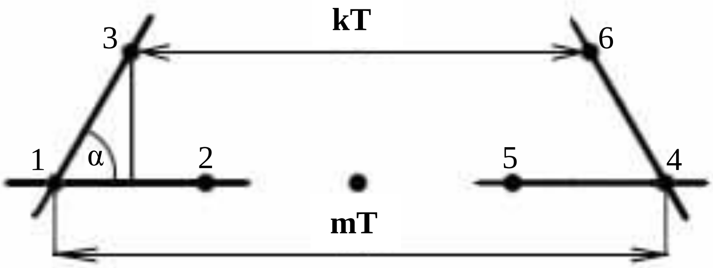
Derivation of types of rotation axes in crystal structures

(*for better understanding the completion of the full course is recommended*)



Suppose that points 1, 2, …, 5, 4 are translationally equivalent. The distance between points 1 and 4 is equal to mT, where T is the length of translation and m is the number of translations.

Suppose that an n-fold rotation axis goes through the point 1 perpendicular to the plane of the picture. Rotating the point 2 counterclockwise around that axis on an angle α one can derive the point 3.

As the point 4 is translationally equivalent with the point 1, the n-fold rotation axis goes through the point 4 the same way, as through the point 1. Rotating the point 5 clockwise (rotation axes can rotate in both directions) around that axis on the same angle α one can derive the point 6.

As points 3 and 6 were derived from translationally equivalent points by the action of the same symmetry operation, they are also translationally equivalent. Thus, points 3 and 6 are located at the distance of the whole number of translations kT from each other.

m, k – whole numbers.
$mT - 2T\cos\alpha = kT$
$m - 2\cos\alpha = k$
$2\cos\alpha = m - k$, thus, $2\cos\alpha$ is a whole number.
$2\cos\alpha = z$, where z is a whole number.
$\cos\alpha = z / 2$
$|\cos\alpha| \le 1$, consequently, $|z / 2| \le 1$, $|z| \le 2$.

Let's analyze all the possible values of z and the corresponding values of angles α and the types of rotation axes n.

z	-2	-1	0	1	2
cosα	-1	-1/2	0	1/2	1
angle α	180°	120°	90°	60°	0° ≡ 360°
axis n	2	3	4	6	1

Thus, only five types of rotation axes are possible in crystal structures:
1, 2, 3, 4, 6.