Zone Axes and the Zone Law

Any two nonparallel planes will intersect in a line; in a crystal, each member of a set of planes ($h_1k_1l_1$) will intersect each member of a nonparallel set of planes ($h_2k_2l_2$) along parallel lines with direction [uvw] where

$$\mathbf{u = k_1l_2 - l_1k_2}$$
$$\mathbf{v = l_1h_2 - h_1l_2}$$
$$\mathbf{w = h_1k_2 - k_1h_2}$$

[uvw] is known as the "zone axis" of these two sets of planes.

(Note: this looks like a vector product, and that is a useful way to remember these relationships, but we are not restricting our discussion to Cartesian coordinates, so the result above is more general).

The planes of a zone axis [uvw] must satisfy the **Weiss Zone Law**:

$$\mathbf{hu + kv + lw = 0}$$

Again, this expression is usually introduced (and utilized) in cubic systems where it can be expressed as the scalar (dot) product of [uvw] and the plane normal [hkl]. But the Weiss zone law also applies in the form above to all lattices, Cartesian or not. Recall that only in cubic systems is [hkl] always the normal to the set of planes (hkl).

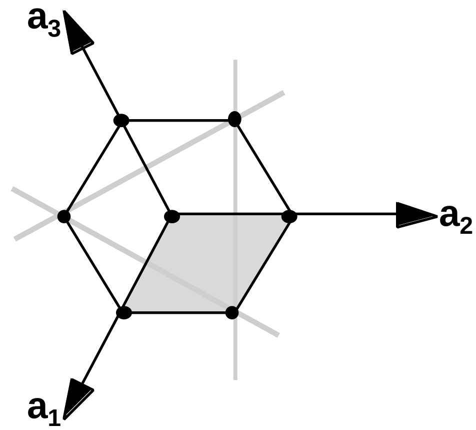
Miller-Bravais Notation

In the description of the five plane lattices, we chose to describe the diamond primitive lattice in terms of a centered rectangular (nonprimitive) lattice. We adopt this convention because the centered rectangle illustrates the rotational symmetry of the lattice more clearly than the diamond lattice. Of course, the downside is that we must be careful in accounting for the two lattice points per cell when we try to describe a pattern or crystal with a centered rectangular lattice. For the same reason, a variation on Miller indices, the Miller-Bravais notation, is often used for hexagonal crystals [and rhombohedral (a.k.a. trigonal) crystals as well]. This 4-index notation (hkil) possesses the apparent symmetry of the hexagonal lattice in the basal plane (the plane perpendicular to the six-fold rotation axes). In other words, M-B notation ascribes similar indices to similar planes.

In the figure below, the primitive 120°-rhombus cell in the basal plane of a hexagonal lattice is shaded. This basal plane of the lattice is fully described by the two basis vectors $\mathbf{a_1}$ and $\mathbf{a_2}$. Of course, $\mathbf{a_3}$ is a crystallographically equivalent basis vector, it is simply redundant.

Exercise: To see why a four index notation is useful for a 3-D hexagonal lattice, write the Miller and M-B indices for each of the three planes (actually members of three sets of planes, to be precise), shown below.

Note that, in M-B, notation: i = - (h + k).

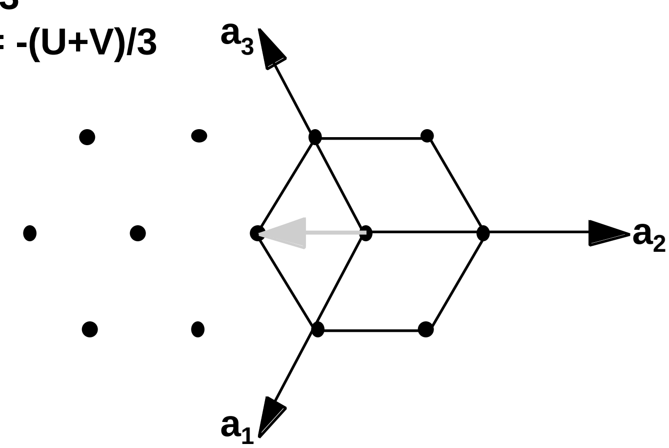


Directions in 4-index Notation

Directions in 4-index notation are less transparent in their construction. Nevertheless, they also display the symmetry of the hexagonal lattice:

If [UVW] is a direction in three-index notation, [uvtw] is the same direction in four-index notation, where:

u = (2U-V)/3
v = (2V-U)/3
t = -(u+v) = -(U+V)/3
w=W



Improper Rotation Axes

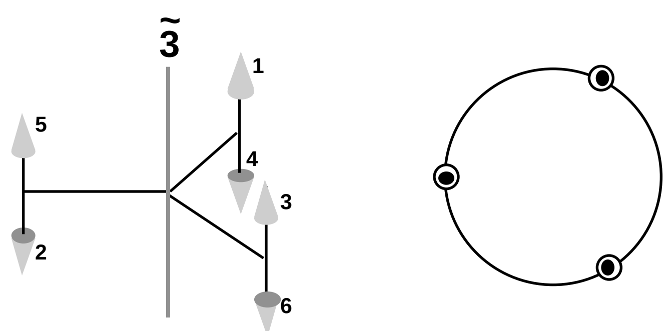
In 3-D, we must consider new classes of point symmetry operations that are not required in 2-D. These compound operations are the combinations of rotation axes with a perpendicular mirror or inversion. [Inversion takes a locus of points L(x,y,z) to a locus of points described by L'(-x,-y,-z). Note that inversion symmetry in 2-D is equivalent to a 2-fold rotation (no change in handedness)].

All of the rotation axes that we have discussed so far are **proper axes**; that is, they generate a sequence of objects, all with the same handedness. An **improper axis** produces objects of alternating handedness. In 2-d, the only improper symmetry operation is the mirror line, which generates enantiomorphs. In 3-d, we also have **rotoreflection** and **roto-inversion**.

Rotoreflection

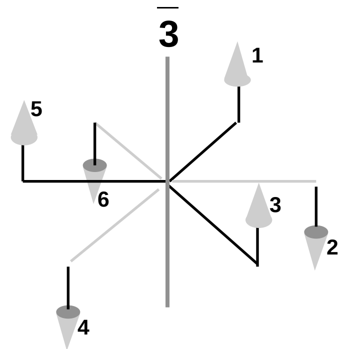
Rotoreflection axes combine rotation with reflection across a mirror plane that is perpendicular to the rotation axis. They are compound symmetry elements. As with the glide mirror, which cannot be decomposed into a simple mirror and a pure translation, a rotoreflection axes is not necessarily equivalent to a proper rotation plus a perpendicular mirror. The first operation takes an object (motif) to an auxilliary (temporary) position and the second operation takes the object to its final position. The operation of an n-fold rotoreflection axis (designated by a tilde: ~) can be described by a counterclockwise rotation by $2\pi/n$, followed by reflection across a perpendicular mirror. This compound operation is repeated until the original object is reproduced. If n is even, this will require n operations; if n is odd, 2n steps will be required to regenerate the initial object. The figure below illustrates the operation of a 3-fold rotoreflection axis. Starting with the arrow #1 pointing up (shown by a black dot in the right-hand figure), the first operation of the rotoreflection axis generates arrow #2 pointing down (illustrated by an open circle in the right-hand figure). The sixth successive operation returns the object to its initial position.

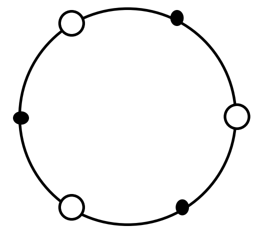
e.g.: $\tilde{3}$



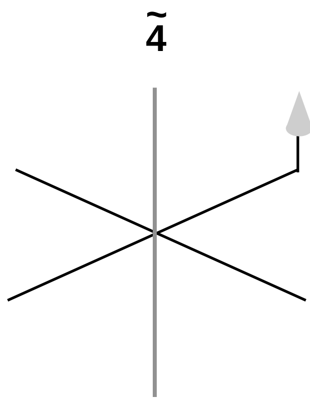
Roto-inversion

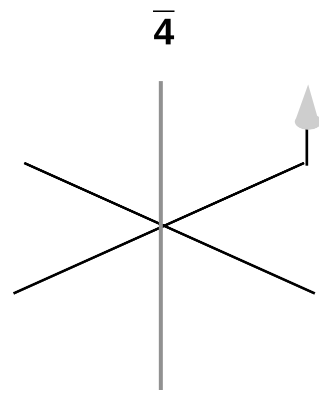
Roto-inversion is analogous to rotoreflection. The compound operation involves rotation and inversion. The overbar is used to designate roto-inversion. The figure below shows the operation of a 3-fold roto-inversion axis.





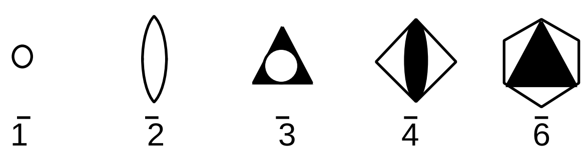
Exercise: apply the four-fold roto-reflection and roto-inversion axes to the arrow motif in the figure below.





Exercise: Considering only rotation axes consistent with translational symmetry, show that all but one of the improper axes can be decomposed into combinations of proper rotations, mirror planes and inversion centers.

The exercise above shows that only the four-fold roto-inversion (or rotoreflection) axis cannot be decomposed into proper rotations, simple mirrors or inversion centers. Nevertheless, you will occasionally see symbols for the other roto-inversion axes as shown below:



In particular, since the 3-fold roto-inversion operation is equivalent to a three fold axis and an inversion center, the symbol for the three-fold roto-inversion axis is often used in tables of point groups and space groups.