MORE ABOUT LATTICES

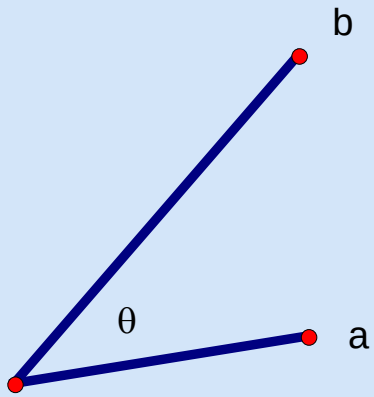
I. The reciprocal lattice

II. The “crystallographic restriction”

III. Lattices and groups

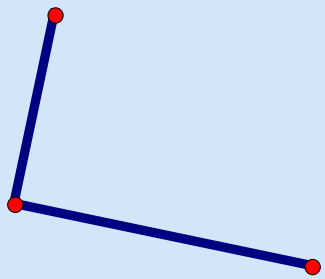
I. The reciprocal lattice

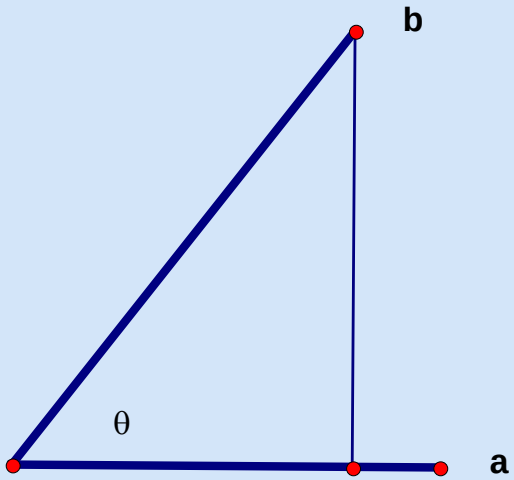
vector scalar products (dot product)



$$a \circ b = |a|\,|b| \cos(\theta)$$

Notice: **a** ◦ **b** = 0 if and only if **a** and **b** are perpendicular.





p = projection of **b** onto **a**

$|p|/|\mathbf{b}| = \cos(\theta)$

$|p| = |\mathbf{b}| \cos(\theta)$

$|a|\ |b| \cos(\theta)$

= |a| x length of the projection of b onto a

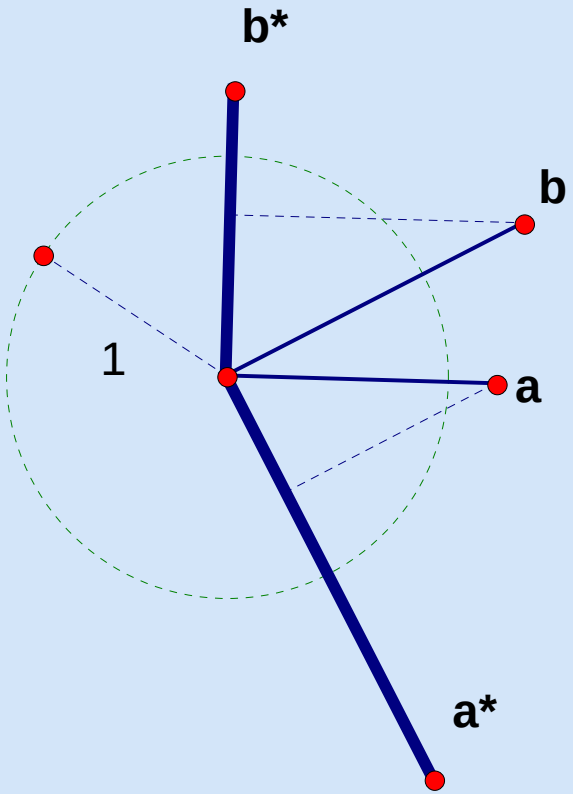
= |b| x length of the projection of a onto b

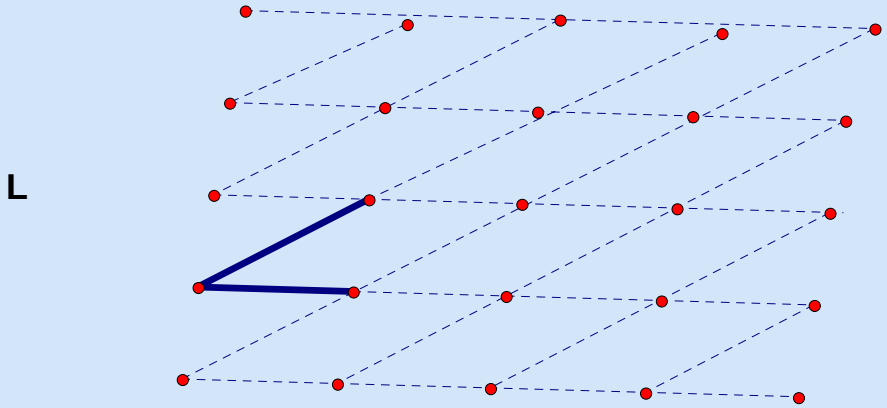
For a lattice L, with basis vectors **a** and **b**, the vectors **a*** and **b*** defined by

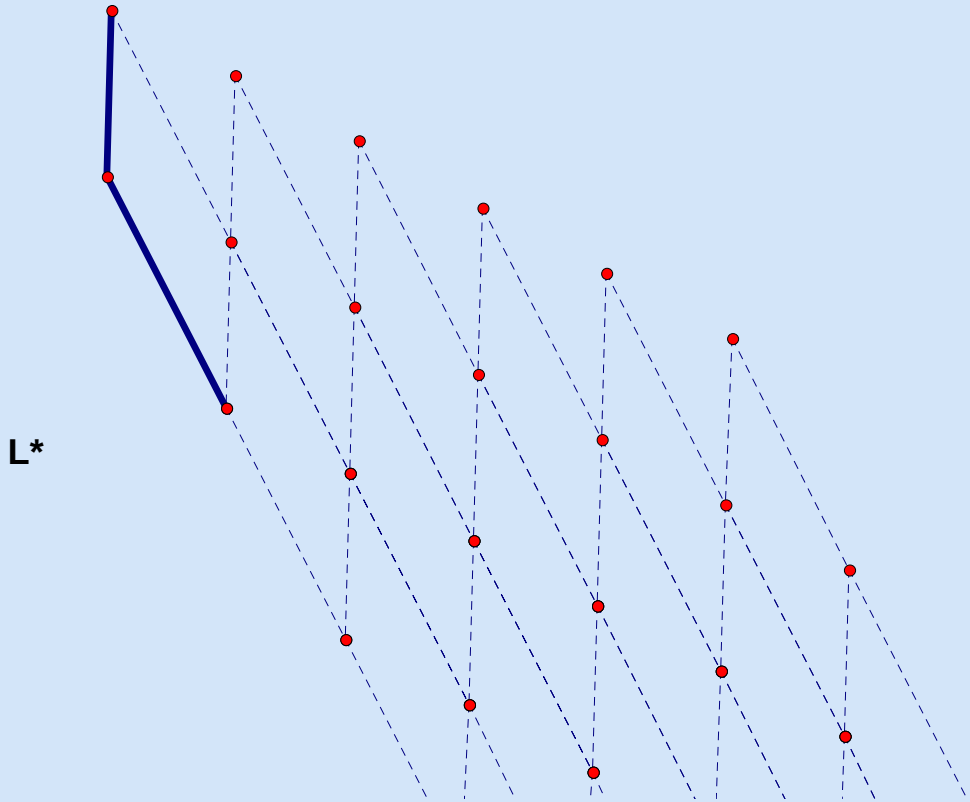
$$\mathbf{a} \circ \mathbf{b}^* = \mathbf{a}^* \circ \mathbf{b} = 0$$

$$\mathbf{a} \circ \mathbf{a}^* = \mathbf{b} \circ \mathbf{b}^* = 1$$

define a lattice L* called the *reciprocal lattice* of L.




L


L*

place in these lectures, but the figure given is sufficiently instructive for our purpose.

Fig. 27 shows an actual X-ray photograph made by passing a fine beam of X-rays through a fixed crystal of 'Iceland spar' (calcium carbonate), about $\frac{1}{4}$ mm. thick.

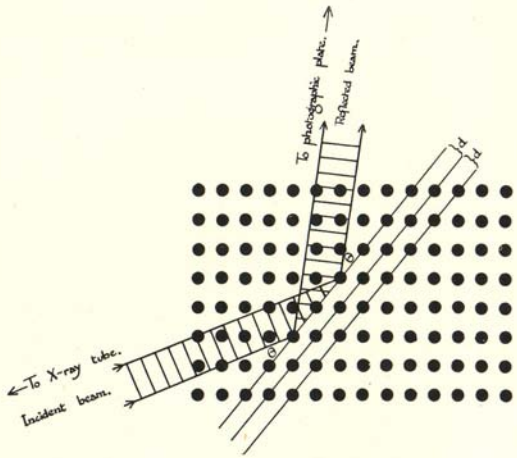


FIG. 26. Illustrating the reflection of an X-ray beam by a layer of molecules in the body of a crystal.

This kind of crystal photograph is called a 'Laue photograph', after the German physicist who first discovered the reflection of X-rays by such means. The experimental arrangement, reduced to its simplest terms, is shown in Fig. 28, the X-ray beam being $\frac{1}{2}$ mm. thick and the distance of the crystal from the photographic plate or film being (for this particular photograph) 2 cm.

Since a parallel beam of X-rays cannot be obtained by the use of a system of glass lenses as is customary with visible light, we are obliged to resort to the use of a 'slit', in this case simply a long narrow tunnel drilled through a piece of dense metal, or two pin-holes, one in each of

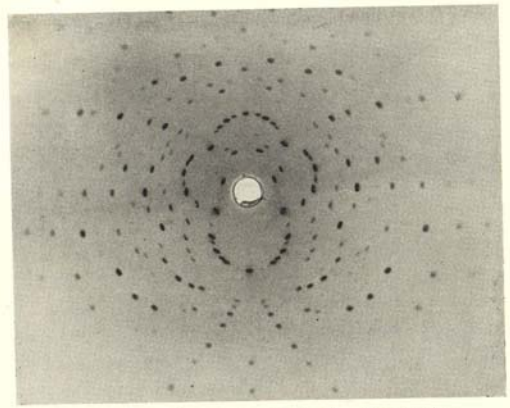


FIG. 27. Laue photograph of 'Iceland spar' ('calcite', or calcium carbonate, $CaCO_3$).

two sheets of lead about 2 inches apart. The dense metal stops all the X-rays except the fine and approximately parallel pencil which is defined by the tunnel or the two pin-holes.

The photographic plate is perpendicular to the X-ray beam, which passes right through the crystal and would strike the plate at its centre were it allowed to do so. In practice such a possibility is carefully guarded against, otherwise the beam would produce at the centre of the

L* is the diffraction pattern of a lattice L.

Lattice vector $\mathbf{t} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$, x,y,z whole numbers

Reciprocal lattice vector $\mathbf{t^*} = h\mathbf{a^*} + k\mathbf{b^*} + l\mathbf{c^*}$, ditto

$$\mathbf{t^*} \circ \mathbf{t} = (\mathbf{t^*} = h\mathbf{a^*} + k\mathbf{b^*} + l\mathbf{c^*}) \circ (x\mathbf{a} + y\mathbf{b} + z\mathbf{c})$$

$$= h\,\mathbf{a^*} \circ x\mathbf{a} + k\mathbf{b^*} \circ y\mathbf{b} + l\mathbf{c^*} \circ z\mathbf{c}$$

$$= hx + ky + lz$$

When $\mathbf{t^*} \circ \mathbf{t} = 0$, $hx + ky + lz = 0$,

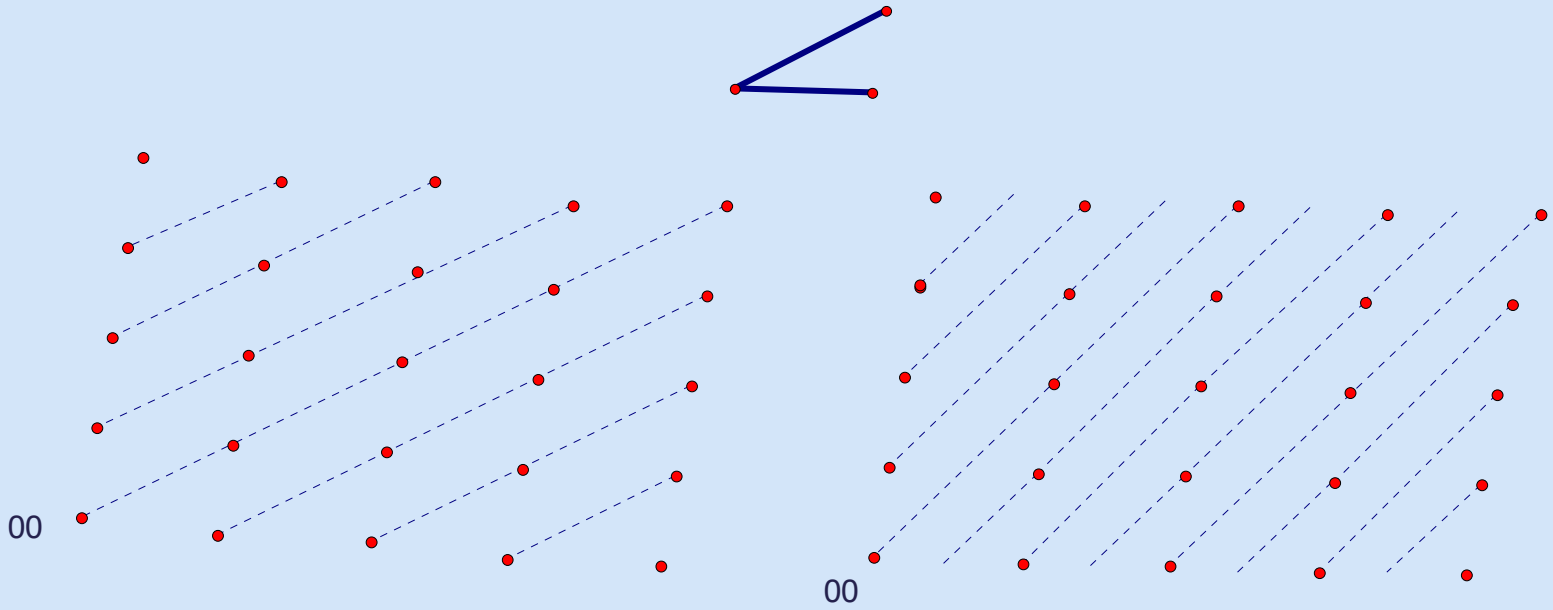
which is the equation of the lattice plane (of L) through the origin perpendicular to $\mathbf{t^* = [hkl]}$

The lattice planes of L perpendicular to the vector **t*** = [hkl] in L* have equations

$$hx + ky + lz = \text{whole number}$$

and the coordinates of the lattice points in those planes, expressed in terms of **a**, **b**, and **c**, are triples xyz, where x,y, and z are whole numbers satisfying the equation.

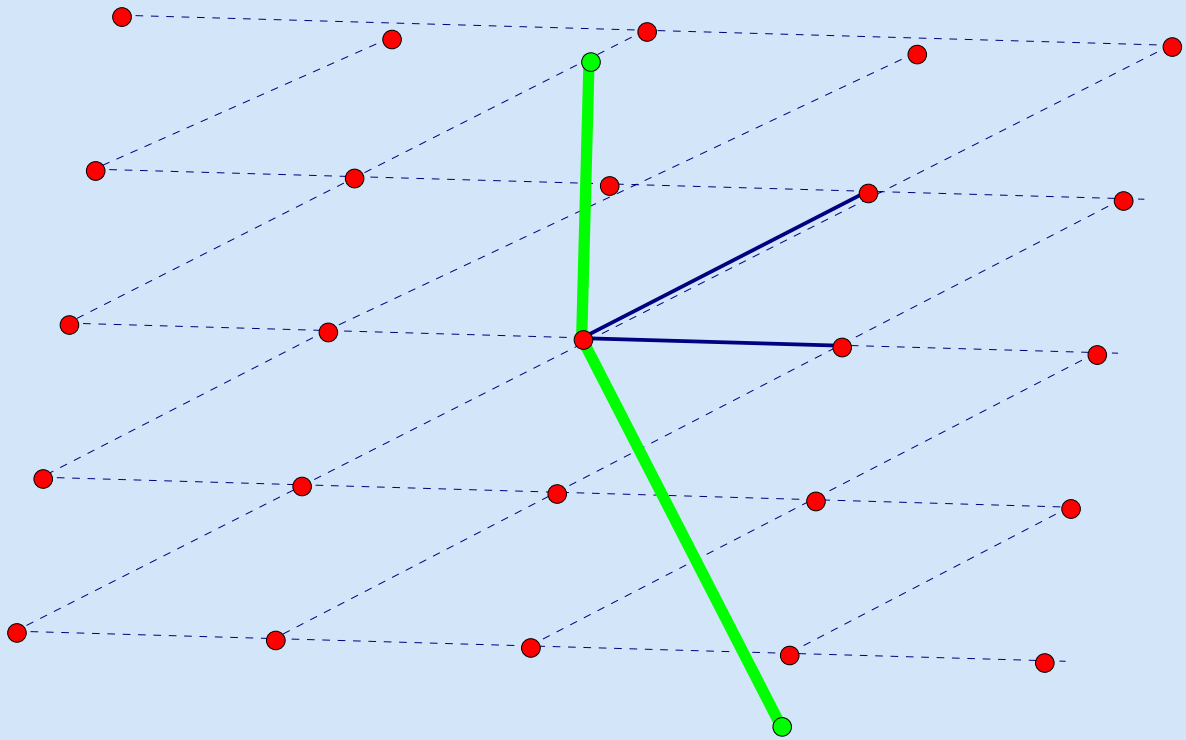
For every **t*** in L, each point of L lies in one of these planes.



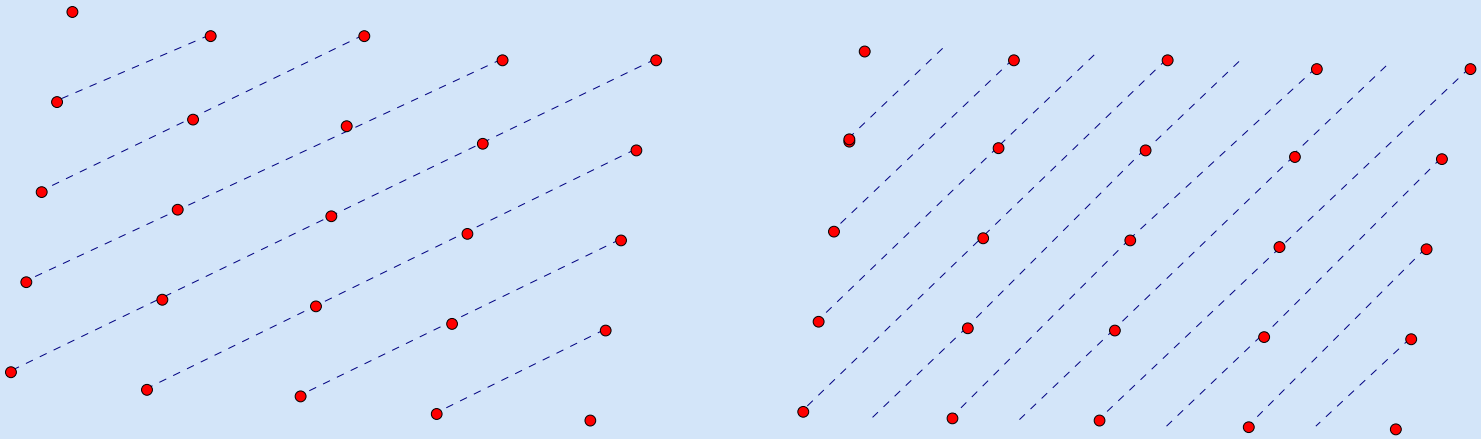
The distance d between two successive lattice planes is the projection of a point in that plane onto the reciprocal lattice vector [hkl] perpendicular to it.

And a little algebra shows that 1/|[hkl]| = d.

That is, the length of a reciprocal lattice vector t* is 1/distance between the lattice points perpendicular to it.



The greater the interplanar spacing, the shorter the reciprocal lattice vector in the perpendicular direction.



Notice that the **greater** the distance between planes,

the **denser** the distribution of lattice points in the planes.

Can we predict the shape of a crystal from its lattice?

Bravais' "Law of Reticular Density"

The faces that appear on a crystal will be parallel to the lattice planes with greatest density.

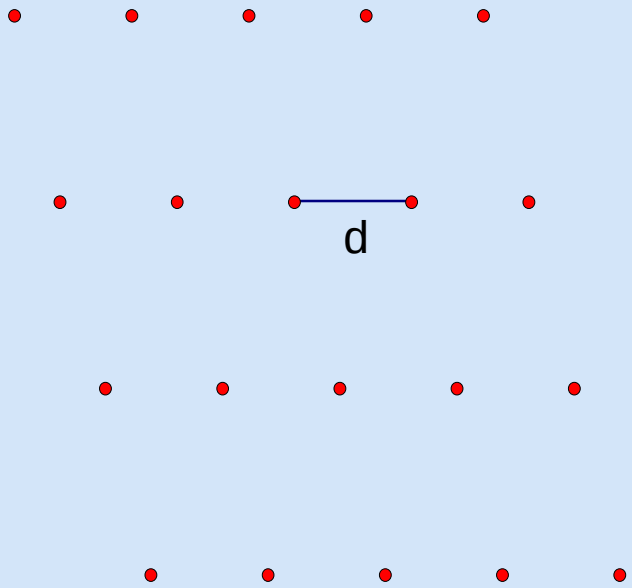
That is, they will be parallel to the lattice planes with largest interplanar distances.

Which means with shortest reciprocal lattice vectors.

Thus, according to Bravais, ***the crystal will have the shape of the Voronoi cell of the reciprocal lattice***.

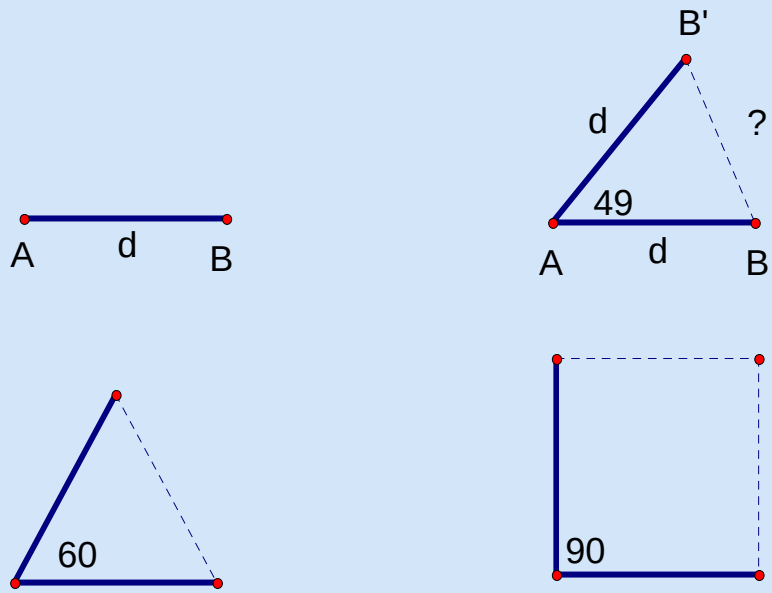
And this agrees with reality surprisingly well!

II. The so-called crystallographic restriction



d is the minimum distance between pairs of points in the lattice

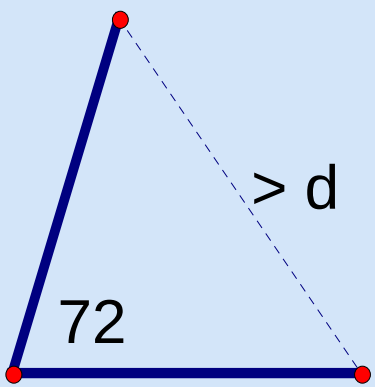
If A and B are lattice points, and we rotate B around A to lattice point B', the distance between B and B' cannot be less than d.



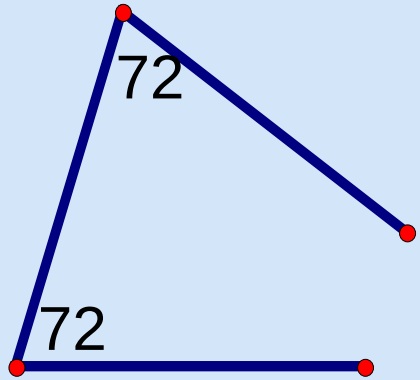
Thus the angle of rotation must be at least 60 degrees.

Which means the rotation can only be 2-,3-,4-,5- or 6- fold.

However, successive 5-fold rotations imply a contradiction.



BUT

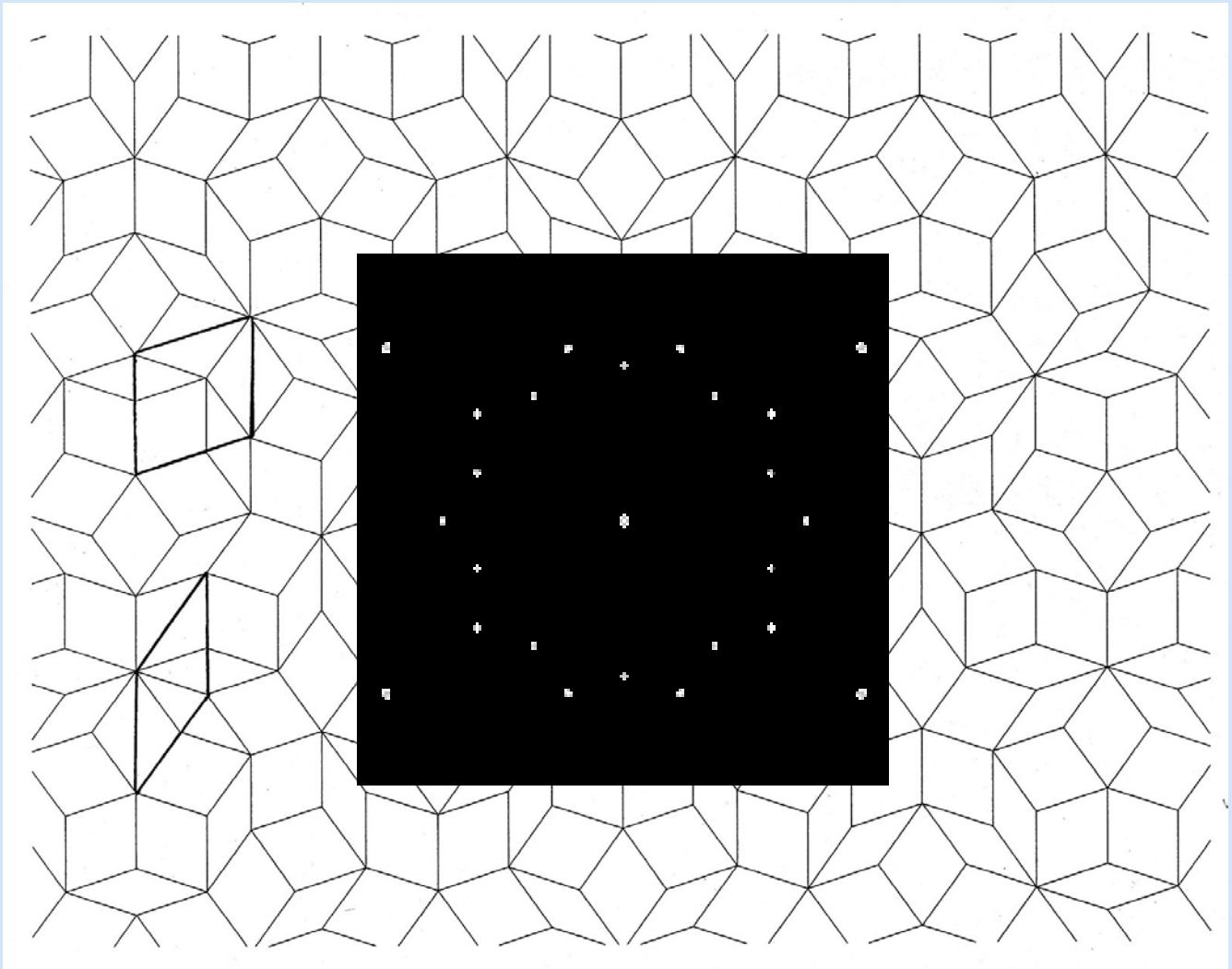


!!!!!

So 5-fold rotation is impossible in a 2D or 3D lattice!

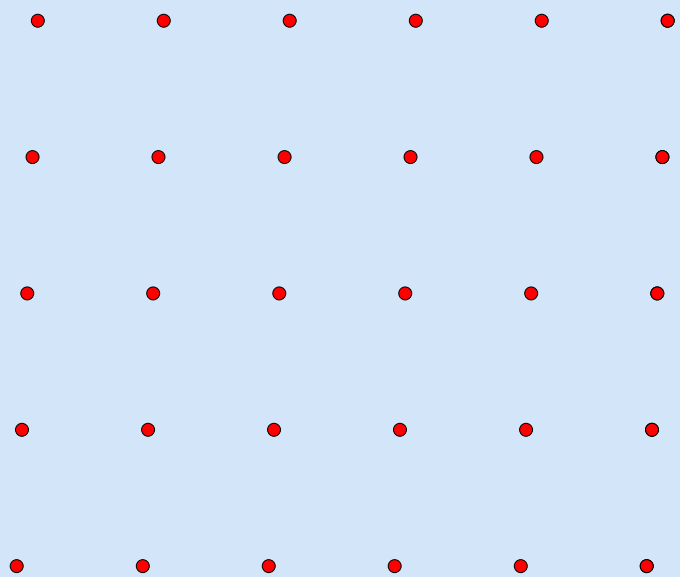
So are 7-, 8-, ... fold rotations. The only possibilities are 2, 3, 4, and 6.

This is the so-called “crystallographic restriction.”



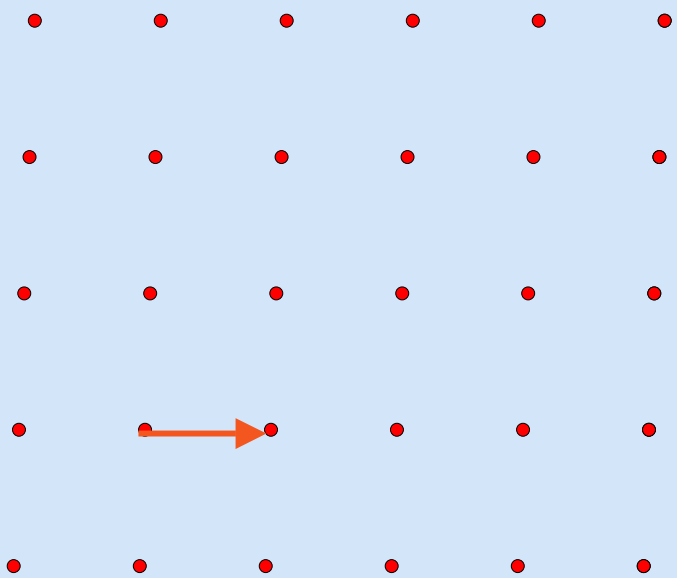
But, it turns out, the “crystallographic restriction” is a theorem about lattices, not a law of nature.

III. Lattice groups

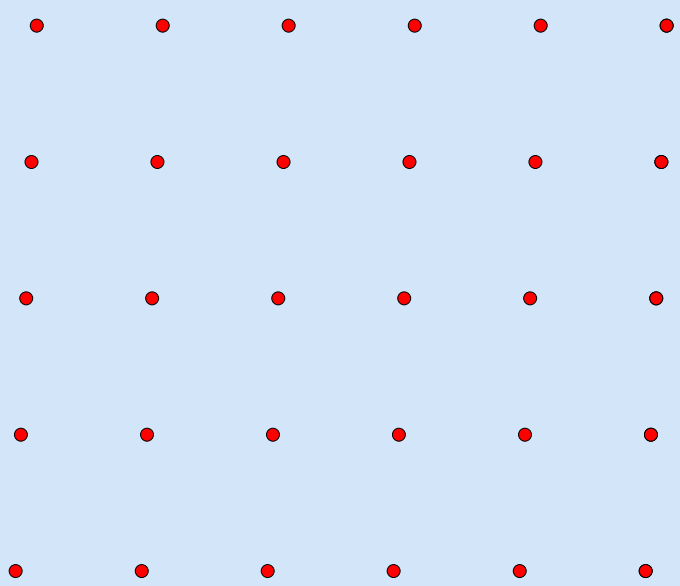


The symmetry group G of a lattice includes translations and rotations, and in some cases reflections and other operations.

The subgroup T of translations (*all* the translations) is a normal subgroup of G.



(A subgroup generated by fewer than n independent translations is *not* necessarily normal.)



The site-symmetry groups S of lattice points are subgroups of G.

These subgroups are conjugate.

The number of cosets of T in G is |S|, the order of the site-symmetry groups S.

Thus the *point group* P = G/T is a group of order |S|, and G is a semi-direct product of T and S.