MORE ABOUT LATTICES

I. The reciprocal lattice
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III. Lattices and groups
I. The reciprocal lattice

vector scalar products (dot product)

\[ a \cdot b = |a| |b| \cos(\theta) \]

Notice: \( a \cdot b = 0 \) if and only if \( a \) and \( b \) are perpendicular.
\[ \cos(\theta) = \frac{\text{length of the projection of } b \text{ onto } a}{|a|} = \frac{|p|}{|b|} \]

\[ |p| = |b| \cos(\theta) \]

\[ |a| \cdot |b| \cos(\theta) = |a| \times \text{length of the projection of } b \text{ onto } a \]

\[ = |b| \times \text{length of the projection of } a \text{ onto } b \]
For a lattice $L$, with basis vectors $a$ and $b$, the vectors $a^*$ and $b^*$ defined by

$$a \cdot b^* = a^* \cdot b = 0$$
$$a \cdot a^* = b \cdot b^* = 1$$

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

![Diagram of lattice and reciprocal lattice](image)
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

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

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

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 \( \mathbf{t}^* = [hkl] \) in \( \mathbf{L}^* \) have equations

\[
hx + ky + lz = \text{whole number}
\]

and the coordinates of the lattice points in those planes, expressed in terms of \( \mathbf{a}, \mathbf{b}, \) and \( \mathbf{c} \), are triples \( \mathbf{xyz} \), where \( x,y, \) and \( z \) are whole numbers satisfying the equation.

For every \( \mathbf{t}^* \) in \( \mathbf{L} \), each point of \( \mathbf{L} \) 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 $1/|\text{[hkl]|} = d$.

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

\[ d \]

\[ d \text{ is the minimum distance between pairs of points in the lattice} \]
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.

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 $S$. 