1.4: Direct and reciprocal lattices

Let's start with a summary of several concepts seen in previous chapters...

Any repetitive and periodic distribution of a ***set of objects*** (or ***motifs***) can be characterized, or described, by translations that repeat the set of objects periodically. The implied translations generate what we call a ***direct lattice*** (or ***real lattice***).

Left: *Fragment of a distribution of a set of objects that produce a direct lattice in 2 dimensions. As an example, one of the infinite sets of motifs (small tiles) that produce the repetitive and periodic distribution is shown inside the yellow squares. The dimensions of the yellow square represent the translations of the direct lattice*

Right: *Fragment of a mosaic in* ***La Alhambra*** *showing a 2-dimensional periodic pattern. These periodic translations can be discovered in the mosaic and produce a 2-dimensional direct lattice. The red square represents the translations of the smallest direct lattice produced by the periodic distributions of the small pieces of this mosaic.The yellow square represents another possible lattice, a bigger one, non primitive.*

Periodic stacking of balls, producing a 3-dimensional network (direct lattice). The motif being repeated in the three directions of space is the contents of the small box with blue edges, the so called "unit cell".

The translations that describe the periodicity in crystals can be expressed as a linear combination of three basic translations, not coplanar, ie independent, known as ***reticular or lattice axes*** (or unit cell axes). These axes define a parallelogram (in 2 dimensions), or a parallelepiped (in 3 dimensions) known as a ***unit cell*** (or elementary cell). This elementary area (in 2-dimensional cases), or elementary volume (in 3-dimensional cases), which holds the minimum set of the periodic distribution, generates (by translations) the full distribution which, in our atomic 3-dimensional case, we call ***crystal***.

In addition to the fact that the ***unit cell*** is the smallest repetitive unit as far as translations is concerned, the reader should note that the system of axes defining the unit cell actually defines the reference system to describe the positional coordinates of each atom within the cell.

Left: *Elementary cell (or unit cell) defined by the 3 non-coplanar reticular translations (cell axes or lattice axes)*

Right: *Crystal formation by stacking of many unit cells in 3 space directions*

In general, inside the unit cell there is a minimum set of atoms (ions or molecules) which are repeated inside the cell due to the **symmetry elements** of the crystal structure. This minimum set of atoms (ions or molecules) which generate the whole contents of the ***unit cell*** (after applying the **symmetry elements** to them) is known as the ***asymmetric unit***.

The structural motif shown in the left figure is repeated by a symmetry element (symmetry operation), in this case a screw axis

The repetition of the motif (asymmetric unit) generates the full content of the unit cell, and the repetition of unit cells generates the entire crystal

The lattice, which is a pure mathematical concept, can be selected in various ways in the same real periodic distribution. However, only one of these lattices "fits" best with the symmetry of the periodic distribution of the motifs...

Two-dimensional periodic distribution of one motif containing two objects (a triangle and a circle)

Left: *Unit cells corresponding to possible direct lattices (=real lattices) that can be drawn over the periodic distribution shown above. Only one of the unit cells (the red one) is more appropriate because it fits much better with the symmetry of the distribution*

Right: *The red cell on the left figure (a centered lattice) fits better with the symmetry of the distribution, and can be decomposed in two identical lattices, one for each object of the motif.*

As is shown in the figures above, although especially in the right one, any lattice that describes the repetition of the ***motif*** (triangle + circle) can be decomposed into two identical equivalent lattices (one for each object of the motif). Thus, the concept of lattice is independent of the complexity of the motif, so that we can use only one lattice, since it represents all the remaining equivalent ones. Once we have chosen a representative lattice, appropriate to the symmetry of the structure, any ***reticular point*** (or ***lattice node***) can be described by a vector that is a linear combination (with integer numbers) of the direct reticular axes: **R = m a + n b + p c**, where **m**, **n** and **p** are integers. ***Non-reticular points*** can be reached using the nearest **R** vector, and adding to it the corresponding fractions of the reticular axes to reach it:

$$\mathbf{r = R + r' = (m a + n b + p c) + (x a + y b + z c)}$$

Position vector for any non-reticular point of a direct lattice

where **x**, **y**, **z** represent the corresponding dimensionless fractions of axes **X/a**, **Y/b**, **Z/c**, and **X**, **Y**, **Z** the corresponding lengths.

Position vector for a non-reticular point (black circle)

The reader should also have a look into the chapters about **lattices** and **unit cells** offered by the University of Cambridge.

Alternatively, the reader can download and run on his own computer **this Java application that illustrates the lattice concept** (it is totally virus free and was developed by Gervais Chapuis and Nicolas Schöni, École Polytechnique Fédérale de Lausanne, Switzerland).

Let's now see some new concepts on direct lattices (= **real lattices) ...**

From a geometric point of view, on a lattice we can consider some ***reticular lines*** and ***reticular planes*** which are those passing through the ***reticular points*** (or reticular nodes). Just as we did with the lattices (choosing one of them from all the equivalent ones), we do the same with the reticular lines and planes. A reticular line or a reticular plane can be used as a representative of the entire family of parallel lines or parallel planes.

Following with the argument given above, each motif in a repetitive distribution generates its own lattice, although all these lattices are identical (**red** and **blue**). Of the two families of equivalent lattices shown (**red** and **blue**) we can choose only one of them, on the understanding that it also represents the remaining equivalent ones. Note that the distance between the planes drawn on each lattice (***interplanar spacing***) is the same for the **blue** or **red** families. However, the family of red planes is separated from the family of blue planes by a distance that depends on the separation between the objects which produced the lattice. This distance between the planes of different families can be called the ***geometric out-of-phase distance***.

Left: *Family of reticular planes cutting the vertical axis of the cell in 2 parts and the horizontal axis in 1 part. These planes are parallel to the third reticular axis (not shown in the figure).*

Right: *Family of reticular planes cutting the vertical axis of the cell in 3 parts and the horizontal axis in 1 part. These planes are parallel to the third reticular axis (not shown in the figure).*

*The number of parts in which a family of planes cut the cell axes can be associated with a triplet of numbers that identify that family of planes. In the three previous figures, the number of cuts, and therefore the numerical triplets would be (**110**), (**210**) and (**310**), respectively, according to the vertical, horizontal and perpendicular-to-the-figure axes. In this figure, the numerical triplets for the planes drawn are (**022**), that is, the family of planes does not cut the **a** axis, but cuts the **b** and **c** axes in **2** identical parts, respectively.*

*The plane drawn on the left side of the figure above cuts the **a** axis in **2** equal parts, the **b** axis in **2** parts and the **c** axis in **1** part. Hence, the numerical triplet identifying the plane will be (**221**). The plane drawn on the right side of the figure cuts the **a** axis into **2** parts, is parallel to the **b** axis and cuts the **c** axis in **1** part. Therefore, the numerical triplet will be (**201**).*

A unique plane, as the one drawn in the top right figure, defined by the numerical triplet known as ***Miller indices***, represents and describes the whole family of parallel planes passing through every element of the motif. Thus, in a crystal structure, there will be as many plane families as possible numerical triplets exist with the condition that these numbers are ***primes***, one to each other (not having a common divisor).

The Miller indices are generically represented by the triplet of letters ***hkl***. If there are common divisors among the Miller indices, the numerical triplet would represent a single family of planes only. For example, the family with indices (***330***), which are not strictly reticular, can be regarded as the representative of **3** families of indices (***110***) with a *geometric out-of-phase distance* (among the families) of **1/3** of the original (see the figures below).

Left: *Three families of reticular planes, with indices (**110**) in three equivalent lattices, showing an out-of-phase distance between them of **1/3** of the interplanar spacing in each family.*

Right: *The same set of planes of the figure on the left drawn over one of the equivalent lattices. Therefore its Miller indices are (**330**) and its interplanar spacing is **1/3** of the interplanar spacing of the (**110**) family.*

Thus, the concept of Miller indices, previously restricted to ***numerical triplets*** (being prime numbers), can now be generalized to ***any triplet of integers***. In this way, every family of planes, will "cover" the whole crystal. And therefore, for every point of the crystal we can draw an infinite number of plane families with infinite orientations.

Through a point in the crystal (in the example in the center of the cell) we can draw an infinite number of plane families with an infinite number of orientations. In this case only 3 families and 3 orientations are shown.

Of course, interplanar spacings can be directly calculated from the Miller indices (***hkl***) and the values of the reticular parameters (unit cell axes). The table below shows that these relations can be simplified for the corresponding metric of the different lattices.

*Formula to calculate the interplanar spacings (d_{hkl}) for a family of planes with Miller indices **hkl** in a unit cell of parameters **a**, **b**, **c**, **α**, **β**, **γ**. Vertical bars (for the triclinic case) mean the function "determinant". In the trigonal case **a**=**b**=**c**=**A**; **α**=**β**=**γ**. In all cases, obviously, the calculated interplanar spacing also represents the distance between the cell origin and the nearest plane of the family.*

Interested readers should also have a look into the chapter on **lattice planes and Miller indices** offered by the University of Cambridge.

And now some more concepts on lattices: the so called **reciprocal lattice ...**

Any plane can also be characterized by a vector (σ_{hkl}) perpendicular to it. Therefore, the projection of the position vector of any point (belonging to the plane), over that perpendicular line is constant and independent of the point. It is the distance of the plane to the origin, ie, the ***spacing*** (d_{hkl}).

Any plane can be represented by a vector perpendicular to it.

Consider the family of planes ***hkl*** with the interplanar distance d_{hkl}. From the set of vectors normal to the planes' family, we take the one (σ_{hkl}) with length $1/d_{hkl}$. The scalar product between this vector and the position vector (d'_{hkl}) of a point belonging to a plane from the family is an integer (n), and this integer gives us the order of that plane in the ***hkl*** family. That is: (σ_{hkl}) . (d'_{hkl}) = ($1/d_{hkl}$) . ($n.d_{hkl}$) = n (see left figure below)

n will be 0 for the plane passing through the origin, 1 for the first plane, 2 for the second, etc.

Thus, σ_{hkl} represents the whole family of ***hkl*** planes having an interplanar spacing given by d_{hkl}. In particular, for the first plane we get: $|\sigma_{hkl}|\ d_{hkl} = 1$.

If we define 1/dhkl, as the length of the vector σ_{hkl}, the product of this vector, times the d_{hkl} spacing of the planes family is the unit.

If we take a vector 2 times longer than σ_{hkl}, the interplanar spacing of the corresponding new family of planes would be a half.

If from this normal vector σ_{hkl} of length $1/d_{hkl}$, we take another vector, n times (integer) longer ($n.\sigma_{hkl}$), the above mentioned product ($|\sigma_{hkl}|\ d_{hkl} = 1$) would imply that the new vector ($n.\sigma_{hkl}$) will correspond to a family of planes of indices ***nh***,***nk***,***nl*** having an interplanar spacing n times smaller. In other words, for instance, the lengths of the following interplanar spacings will bear the relation: $d_{100} = 2.(d_{200}) = 3.(d_{300})$..., so that $\sigma_{100} = (1/2).\sigma_{200} = (1/3).\sigma_{300}$ ... and similarly for other ***hkl*** planes.

Therefore, it appears that the moduli (lengths) of the perpendicular vectors (σ_{hkl}) are ***reciprocal to the interplanar spacings***. The end points of these vectors (blue arrows in figure below) also produce a periodic lattice that, due to this reciprocal property, is known as the ***reciprocal lattice*** of the original direct lattice. The ***reciprocal points*** obtained in this way (green points in figure below) are identified with the same numerical triplets ***hkl*** (***Miller indices***) which represent the corresponding plane family.

*Geometrical construction of some points of a reciprocal lattice (green points) from a direct lattice. To simplify, we assume that the third axis of the direct lattice (**c**) is perpendicular to the screen. The red lines represent the reticular planes (perpendicular to the screen) and whose Miller indices are shown in blue. As an example: the reciprocal point with indices **(3,1,0)** will be located on a vector perpendicular to the plane **(3,1,0)** and its distance to the origin **O** is inversely proportional to the spacing of that family of planes.*

Animated example showing how to obtain the reciprocal points from a direct lattice

It should now be clear that the direct lattice, and its reticular planes, are directly associated (linked) with the ***reciprocal lattice***. Moreover, in this reciprocal lattice we can also define a unit cell (***reciprocal unit cell***) whose periodic translations will be determined by three ***reciprocal axes*** that form ***reciprocal angles*** among them. If the unit cell axes and angles of the direct cell are known by the letters ***a***, ***b***, ***c***, ***α***, ***β***, ***γ***, the corresponding parameters for the reciprocal cell are written with the same symbols, adding an asterisk: ***a****, ***b****, ***c****, ***α****, ***β****, ***γ****. It should also be clear that these reciprocal axes (***a****, ***b****, ***c****) will correspond to the vectors σ_{100}, σ_{010} and σ_{001}, respectively, so that any reciprocal vector can be expressed as a linear combination of these three reciprocal vectors:

$$\sigma_{hkl} = h\ a^* + k\ b^* + l\ c^*$$

Position vector of any reciprocal point

Geometrical relation between direct and reciprocal unit cells

The figure below shows again the strong relationship between the two lattices (**direct with blue points**, **reciprocal in green**). In this case, the corresponding third reciprocal axes (**c** and **c***) are perpendicular to the screen.

And analytically the relationship between the direct (= real) and reciprocal cells can be written as:

*Metrical relations among the parameters defining the direct and reciprocal cells. **V** represents the volume of the direct cell and the symbol **x** means the cross product between two vectors. The same type of equations can be written by changing the asterisks to the right side of the equations. The volume of the direct cell can be calculated as:*

$V = (a \times b) \cdot c = a.\ b.\ c\ (1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}$

Note that, in accordance with the definitions given above, the length of a^* is the inverse of the interplanar spacing d_{100} ($|a^*| = 1/d_{100}$), and that $|b^*| = 1/d_{010}$, and that $|c^*| = 1/d_{001}$. Therefore, the following scalar products (dot products) can be written: $a.a^* = 1$, $a.b^* = 0$ and similarly with the other pairs of axes.

Summarizing:

- Direct space (= real space) is the space where we live..., where atoms are..., where crystals growth..., where we imagine the direct lattices (= real lattices).
- Reciprocal space is a mathematical space constructed on the direct space (= real space). It is the space where reciprocal lattices are, which will help us to understand the crystal diffraction phenomena.
- "*Big in direct space (that is, in real space)*", means "*small in reciprocal space*".
- "*Small in direct space (that is, in real space)*" means "*big in reciprocal space*".

In addition to this, we recommend to download and execute the Java applet by Nicolas Schoeni and Gervais Chapuis of the Ecole Polytechnique Fédéral de Lausanne (Switzerland) to **understand the relation between direct and reciprocal lattices and how to build the latter from a direct lattice**. (Free of any kind of virus).

See also the pages on ***reciprocal space*** offered by the **University of Cambridge through this link**.

And although we are revealing aspects corresponding to the next chapter (see the last paragraph of this page), the reader should also **look at the video** made by **www.PhysicsReimagined.com**, showing the geometric relationships between direct and reciprocal lattices, displayed below as an animated gif:

The reader is probably asking himself why we need this new concept (the ***reciprocal lattice***). Well, there are reasons which justify it. One of them is that a *family of planes can be represented by just one point*, which obviously simplifies things. And another important reason is that this new lattice offer us a very simple geometric model that can interpret the ***diffraction*** phenomena in crystals. But this will be described in another chapter. Go on!
