

Crystal Geometry

Bibliography:

Assigned Reading:

[Poirier, 1985]Chapter 2, 4.

General References:

[Kelly and Groves, 1970] Chapter 1.

[Hirth and Lothe, 1982]

Hirth, J.P., and J. Lothe, *Theory of dislocations*, xii, 857 pp., Wiley, New York, 1982.

Kelly, A., and G.W. Groves, *Crystallography and Crystal Defects*, 428 pp., Addison Wesley, N. Y., 1970.

Poirier, J.-P., *Creep of crystals: High-temperature deformation processes in metals, ceramics, and minerals*, 260 pp., Cambridge, 1985.

Lattice points, crystal basis, and crystal lattices:

1. Lattice point: Two equivalent lattice points are points in space for which the surroundings (atomic positions and identities) are identical. Any point in space in the lattice may be chosen as the origin.
2. The chemical surroundings of each lattice point are identical with those of each and every other lattice point.
3. An ensemble of lattice points is a mesh in 2d or a lattice in 3d.
In a 1 mm cube of NaCl (cubic lattice with lattice dimension of 5.64 angstroms), there are about 2 million lattice points in one direction, or about 8×10^{18} lattice points in the cube!
4. The actual disposition of the atoms or ions around each lattice point is called the crystal basis. Depending on the details of the bonding and the crystal chemistry, the crystal basis may contain more than one stoichiometric unit.
5. The actual crystal itself is a combination of the crystal basis and the crystal lattice. The crystal structure is completely defined and represented by repeating the crystal basis at every lattice point.
6. Depending on the geometry and symmetry of the crystal, every crystal lattice can be included within one of seven crystal systems or one of 14 classes represented by unique Bravais crystal space lattices.
7. A vector connecting one lattice point to another is a lattice vector. Because each lattice point repeats at a fixed interval, three non-coplanar vectors are sufficient to span the space of all lattice points in three dimensions. The three smallest vectors are called primitive lattice vectors and define a unit cell, the primitive unit cell, that contains the smallest volume that can be stacked repeatedly to produce the entire crystal. By convention the unit cell is chosen so that the crystallographic axes contain an obtuse angle unless the axes are perpendicular to each other.
8. Every lattice vector may be expressed as a linear combination of an integral number of the primitive unit vectors. Remember that the lattice vectors do not

necessarily form an orthonormal set, that is the lattice vectors are not all the same length and are not necessarily perpendicular to each other.

9. Rational directions are vectors that are composed of integral numbers of lattice vectors. Thus, rational directions always connect one lattice point to another. They are denoted by three numbers within brackets or carets, e.g. $[1\ 5\ 9]$ or $\langle 1\bar{1}\ 0 \rangle$. The latter refers to a set of directions that are symmetrically equivalent. The overscore indicates -1.

Choice of the origin of the lattice vectors is arbitrary, but once chosen, the lengths and angles between the vectors are fixed by the crystal geometry.

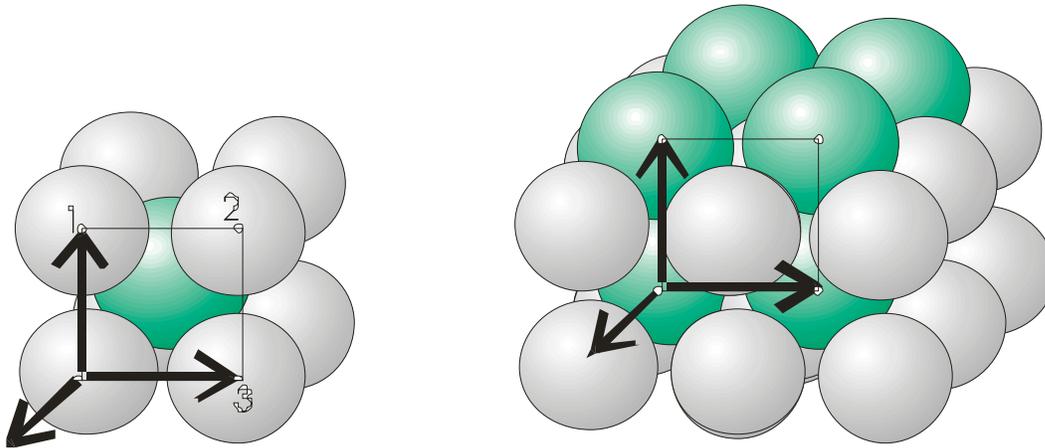
Lattice Coordinates

The symmetry of each lattice point can be represented by one of _____ space groups. The translational symmetry (i.e. the repetition structure of the lattice points) can be categorized as one of seven crystal systems:

Table 1.3 The crystal systems (from Kelly and Grove, 1970)

System	Symmetry (Minimum)	Conventional Cell
Triclinic	No axes of symmetry	$a \neq b \neq c; \alpha \neq \beta \neq \gamma$
Monoclinic	Single diad	$a \neq b \neq c; \alpha = \gamma = 90^\circ < \beta$
Orthorhombic	Three \perp diads	$a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$
Trigonal (Rhombohedral)	Single triad	$a = b = c; \alpha = \beta = \gamma < 120^\circ$
Hexagonal	One hexad	$a = b = c; \alpha = \beta = \gamma < 120^\circ$
Cubic	Four triads	$a = b = c; \alpha = \beta = \gamma = 90^\circ$

Example I): CsCl structure: Cs is the smaller grey ion. Diagram is schematic and not necessarily to scale.



If the origin is chosen as the center of the cesium ion, then the smallest lattice vectors that can be chosen are equal and mutually perpendicular. The crystal system is cubic. The internal coordinates of the Cl in the first choice of lattice vectors are $[\frac{1}{2} \frac{1}{2} \frac{1}{2}]$. The unit cell contains one stoichiometric unit, CsCl. Notice that the lattice vectors and their geometry do not change if the origin is changed.

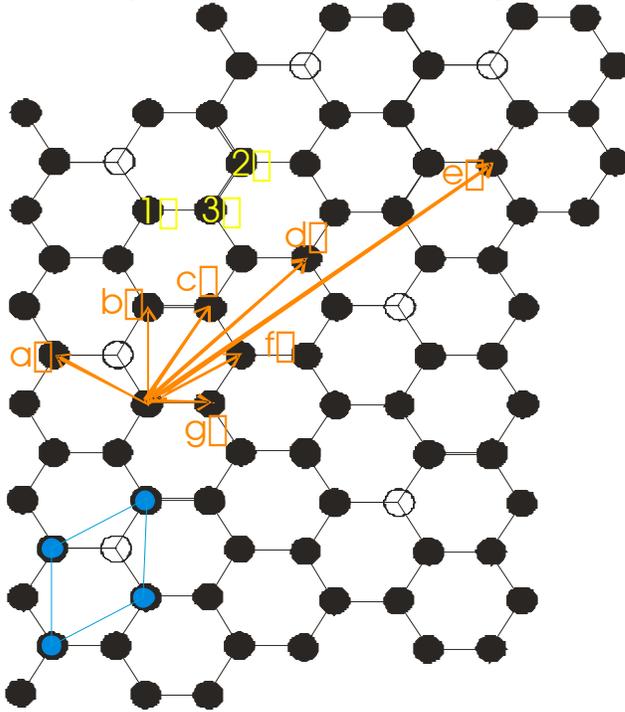
Example II) Graphite mesh

Below is a mesh (a 2D array of lattice points). Clearly, the lattice points have hexagonal symmetry and are similar to the arrangement of atoms in a sheet of graphite.

First, consider atoms, 1, 2 and 3. Are these positions equivalent allowing only translations?

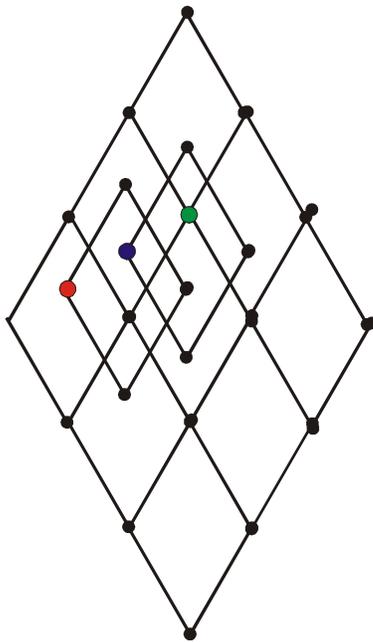
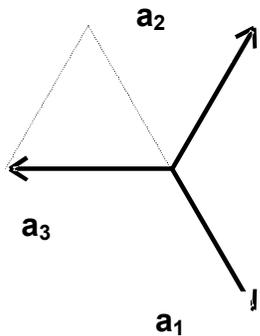
Now consider vectors a-g. Which of these vectors are lattice vectors?

Outlined in blue is the primitive unit cell. The atoms on the corners and contained within the four vectors are the crystal basis. The entire mesh can be generated by translating the unit cell by linear combinations of the primitive unit lattice vectors.



Hexagonal system and Miller-Bravais Indices

Hexagonal system and Miller-Bravais Indices



Hexagonal lattice vectors are equal and at 120° to each other. The third axis extends out of the board [001]

Can define a fourth lattice vector at 120° to the other two in the plane perpendicular to c .

- Can define a set of indices $[u \ v \ t \ w]$
- t is redundant since $u\mathbf{a}_1 + v\mathbf{a}_2 = -t\mathbf{a}_3$
- Result numbers are called *the Miller-Bravais indices*
- Complication is tolerated because the relation between symmetrical directions and planes is more readily apparent.

Word about Relation between Rhombohedral and Hexagonal lattices.

Two lattices are related: rhombohedral is a primitive unit cell in a degenerate hexagonal cell

By stacking a hexagonal mesh in the BA order, we can construct a triply degenerate hexagonal cell.

An example of this sort of chicanery is the rhombohedral and trigonal lattices of calcite.

c axis in hexagonal system is parallel to three fold

Summary: Lattices, Lattice Directions

1. Lattice points: Point in a crystal with specific arrangement of atoms, reproduced many times in the crystal
2. Crystal basis: Arrangement of atoms within the unit cell.
3. Lattice vectors connect two lattice points. There are 14 Bravais lattices included in seven crystal systems. (Triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral-trigonal, hexagonal, and cubic).
4. Any lattice point may be reached from any other by the vector addition of an integral number of lattice vectors.
5. Unit cells are made by defining a set of coordinate axes composed of three non-coplanar, non-colinear lattice vectors.
6. A primitive unit cell contains one lattice point, but may contain many atoms.
7. The preferred unit cell is primitive, has lattice vectors as nearly equal in length as possible, and has an obtuse angle between two vectors, if possible. The preferred setting of the lattice often, but not always, has the symmetry element of greatest rank parallel with the c axis. (The monoclinic and trigonal-rhombohedral lattices are exceptions to this rule.
8. Non-integral combinations of the lattice vectors give the atomic positions of the crystal basis.
9. Lattice directions are specified by (integral) components of the lattice vectors. They are denoted by a triple of numbers contained in brackets like $\langle u \ v \ w \rangle$ for a single direction or $[u \ v \ w]$ for a set of symmetrically equivalent directions.
10. Miller Bravais notation, i.e. $[u \ v \ t \ w]$, is sometimes used for the hexagonal system. The third index, t , is redundant since $u+v-t=0$.

Crystal plane and Miller indices

Summary: Lattices Planes, Crystal Forms, and Reciprocal Lattice

1. Miller Indices arise from finding the plane intercepts, inverting, forming a vector and clearing fractions or common factors
2. The Miller indices are the components of the equation for the plane.
3. Each set of Miller indices represents a set of parallel planes. Indices that are integral multiples of another set are parallel planes with a smaller interplanar spacing e.g. (4 4 2) and (2 2 1).
4. In general a given direction is not parallel to the pole of a plane with the same Miller indices.
5. Equivalent planes may be discovered by examining a stereogram and considering the symmetry elements.
6. Some planes in the crystal (crystal forms) are common enough or important enough to be given special names. The naming can be by Miller indices, classical terminology, by pole symmetry, or be lower case letters.
7. Reciprocal vectors are formed by choosing a vector perpendicular to two lattice vectors and of reciprocal length to the third lattice vector.
8. The lattice formed from these reciprocal vectors has lattice vectors that are in the same direction as the poles to the corresponding planes. The lattice vector length is the reciprocal of the plane spacing.