Crystal structure

(from Wikipedia: http://en.wikipedia.org/wiki/Crystal_structure [1])

Fi.g 1 Enargite crystals

In mineralogy and crystallography, a **crystal structure** is a unique arrangement of atoms in a crystal. A crystal structure is composed of a **unit cell**, a set of atoms arranged in a particular way; which is periodically repeated in three dimensions on a lattice. The spacing between unit cells in various directions is called its *lattice parameters.* The symmetry properties of the crystal are embodied in its space group. A crystal's structure and symmetry play a role in determining many of its properties, such as cleavage, electronic band structure, and optical properties.

Unit cell

The crystal structure of a material is often discussed in terms of its unit cell. The unit cell is a spatial arrangement of atoms which is tiled in three-dimensional space to describe the crystal. The unit cell is given by its lattice parameters, the length of the cell edges and the angles between them, while the positions of the atoms inside the unit cell are described by the set of atomic positions (x_i,y_i,z_i) measured from a lattice point.

For each crystal structure there is a *conventional unit cell,* which is the smallest unit that has the *full symmetry* of the crystal (see below). However, the conventional unit cell is not always the smallest possible choice. A **primitive unit cell** of a particular crystal structure is the smallest possible unit cell one can construct such that, when tiled, it completely fills space. This primitive unit cell does not, however, display all the symmetries inherent in the crystal. A Wigner-Seitz cell is a particular kind of primitive cell which has the same symmetry as the lattice.

Classification of crystals by symmetry

The defining property of a crystal is its inherent symmetry, by which we mean that under certain *operations* the crystal remains unchanged. For example, rotating the crystal 180 degrees about a certain axis may result in an atomic configuration which is identical to the original configuration. The crystal is then said to have a two-fold rotational symmetry about this axis. In addition to rotational symmetries like this, a crystal may have symmetries in the form of mirror planes and

translational symmetries, and also the so-called *compound symmetries* which are a combination of translation and rotation/mirror symmetries. A full classification of a crystal is achieved when all of these inherent symmetries of the crystal are identified.

Crystal system

The crystal systems are a grouping of crystal structures according to the axial system used to describe their lattice. Each crystal system consists of a set of three axes in a particular geometrical arrangement. There are seven unique crystal systems. The simplest and most symmetric, the cubic (or isometric) system, has the symmetry of a cube, that is, the three axes are mutually perpendicular and of equal length. The other six systems, in order of decreasing symmetry, are hexagonal, tetragonal, rhombohedral (also known as trigonal), orthorhombic, monoclinic and triclinic. Some crystallographers consider the hexagonal crystal system not to be its own crystal system, but instead a part of the trigonal crystal system. The crystal system and Bravais lattice of a crystal describe the (purely) translational symmetry of the crystal.

The Bravais lattices

When the crystal systems are combined with the various possible lattice centerings, we arrive at the Bravais lattices. They describe the geometric arrangement of the lattice points, and thereby the translational symmetry of the crystal. In three dimensions, there are 14 unique Bravais lattices which are distinct from one another in the translational symmetry they contain. All crystalline materials recognized until now (not including quasicrystals) fit in one of these arrangements. The fourteen three-dimensional lattices, classified by crystal system, are shown in Table 1. The Bravais lattices are sometimes referred to as *space lattices*.

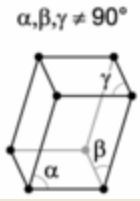
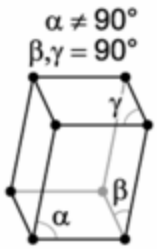
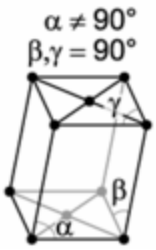
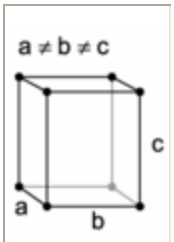
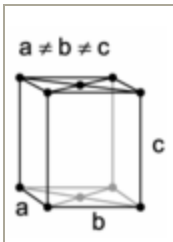
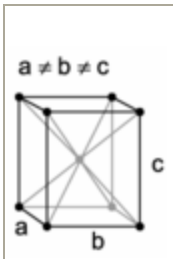
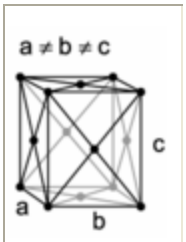
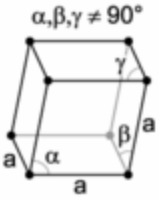
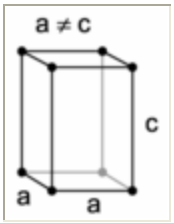
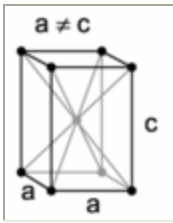
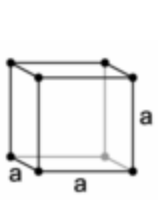
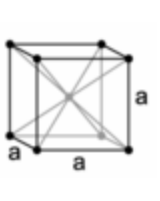
The crystal structure consists of the same group of atoms, the *basis*, positioned around each and every lattice point. This group of atoms therefore repeats indefinitely in three dimensions according to the arrangement of one of the 14 Bravais lattices. The characteristic rotation and mirror symmetries of the group of atoms, or unit cell, is described by its crystallographic point group.

Point and space groups

The crystallographic point group or *crystal class* is the set of non-translational symmetry operations that leave the appearance of the crystal structure unchanged. These symmetry operations can include *mirror planes*, which reflect the structure across a central plane, *rotation axes*, which rotate the structure a specified number of degrees, and a *center of symmetry* or *inversion point* which inverts the structure through a central point. There are 32 possible crystal classes. Each one can be classified into one of the seven crystal systems.

The [space group](#) of the crystal structure is composed of the translational symmetry operations in addition to the operations of the point group. These include pure *translations* which move a point along a vector, *screw axes*, which rotate a point around an axis while translating parallel to the axis, and *glide planes*, which reflect a point through a plane while translating it parallel to the plane. There are 230 distinct space groups.

Table 1. Crystal Structures

Crystal system	Lattices			
[triclinic](#)				
[monoclinic](#)	simple	base-centered		
				
[orthorhombic](#)	simple	base-centered	body-centered	face-centered
				
[hexagonal](#)				
[rhombohedral](#) (trigonal)				
[tetragonal](#)	simple	body-centered		
				
[cubic](#) (isometric)	simple	body-centered	face-centered	
				

Physical properties

Defects in crystals

Real crystals feature defects or irregularities in the ideal arrangements described above and it is these defects that critically determine many of the electrical and mechanical properties of real materials. In particular dislocations in the crystal lattice allow shear at much lower stress than that needed for a perfect crystal structure.

Crystal symmetry and physical properties

Twenty of the 32 crystal classes are so-called piezoelectric, and crystals belonging to one of these classes (point groups) display piezoelectricity. All 20 piezoelectric classes lack a center of symmetry. Any material develops a dielectric polarization when an electric field is applied, but a substance which has such a natural charge separation even in the absence of a field is called a polar material. Whether or not a material is polar is determined solely by its crystal structure. Only 10 of the 32 point groups are polar. All polar crystals are pyroelectric, so the 10 polar crystal classes are sometimes referred to as the pyroelectric classes.

There are a few crystal structures, notably the perovskite structure, which exhibit ferroelectric behaviour. This is analogous to ferromagnetism, in that, in the absence of an electric field during production, the ferroelectric crystal does not exhibit a polarisation. Upon the application of an electric field of sufficient magnitude, the crystal becomes permanently polarised. This polarisation can be reversed by a sufficiently large counter-charge, in the same way that a ferromagnet can be reversed. However, it is important to note that, although they are called ferroelectrics, the effect is due to the crystal structure, not the presence of a ferrous metal.

Incommensurate crystals have period-varying translational symmetry. The period between nodes of symmetry is constant in most crystals. The distance between nodes in an incommensurate crystal is dependent on the number of nodes between it and the base node.

References:

[1] http://en.wikipedia.org/wiki/Crystal_structure