2.CRYSTAL STRUCTURE.

Aim: To obtain an understanding of the concepts used to describe crystal structure as well as knowledge of the lattice types.

The physical properties of solids depend on their structure, i.e. their arrangement of atoms. Therefore it is necessary to understand the various crystal structures before proceeding to physical properties.

A. Concepts, definitions (Kittel (K) p. 3-6).

A **crystal** is a three-dimensional periodic arrangements of atoms in space. We describe it with the use of a mathematical abstraction, the lattice.

A **lattice** is an infinite periodic array of points in space. Its arrangement and orientation appears exactly the same, from whichever of the points it is viewed. The lattice is invariant under translation symmetry.

A group of atoms, a **basis**, may be attached to each lattice point. Hence we can say that lattice+basis = crystal structure.

The lattice can be divided into identical primitive cells. The **primitive cell** is the volume of space associated with one lattice point. The primitive cell can be depicted as a parallelepiped with lattice points in the corners. The edges of the parallelepiped are the **primitive translation vectors** of the lattice. Their magnitudes are the **lattice constants**. More often another type of primitive cell, the **Wigner-Seitz cell**, is used. It is limited by the planes bisecting the lines drawn from a lattice point to its neighbours. A larger **crystallographic unit cell** is sometimes used to display the symmetry of a crystal structure more clearly. Especially in the cubic systems, the lattice constants are often taken as the length of the sides of the crystallographic unit cell.

B. Lattice types (K 6-11).

Apart from the fundamental translation symmetry, a lattice may also exhibit other symmetries:

Rotations by $2\pi/n$ where n=1,2,3,4,6.
Reflection in a plane through a lattice point.
Rotoreflection, i.e. a rotation + a reflection in a plane orthogonal to the rotation axis.
    An example of this is the inversion, by which **r-->-r**.

The different symmetries a lattice can have, leads to a classification in terms of different lattice types or **Bravais lattices**. There are 5 types in two dimensions and 14 ones in three dimensions. The three-dimensional lattice types are illustrated in figure 1, together with some characteristics as well as system names. It is seen that the crystallographic unit cells are given in several cases. The a_i's are the lattice constants, or the side lengths of the crystallographic unit cell. The α,β,γ are the angles defining the shape of the unit cell.

A three-dimensional Bravais lattice consists of all points with position vectors

$$\mathbf{r} = u_1\,\mathbf{a_1} + u_2\,\mathbf{a_2} + u_3\,\mathbf{a_3},$$

Where the u's are integers and the **a**'s denote the primitive translation vectors that generate the lattice.
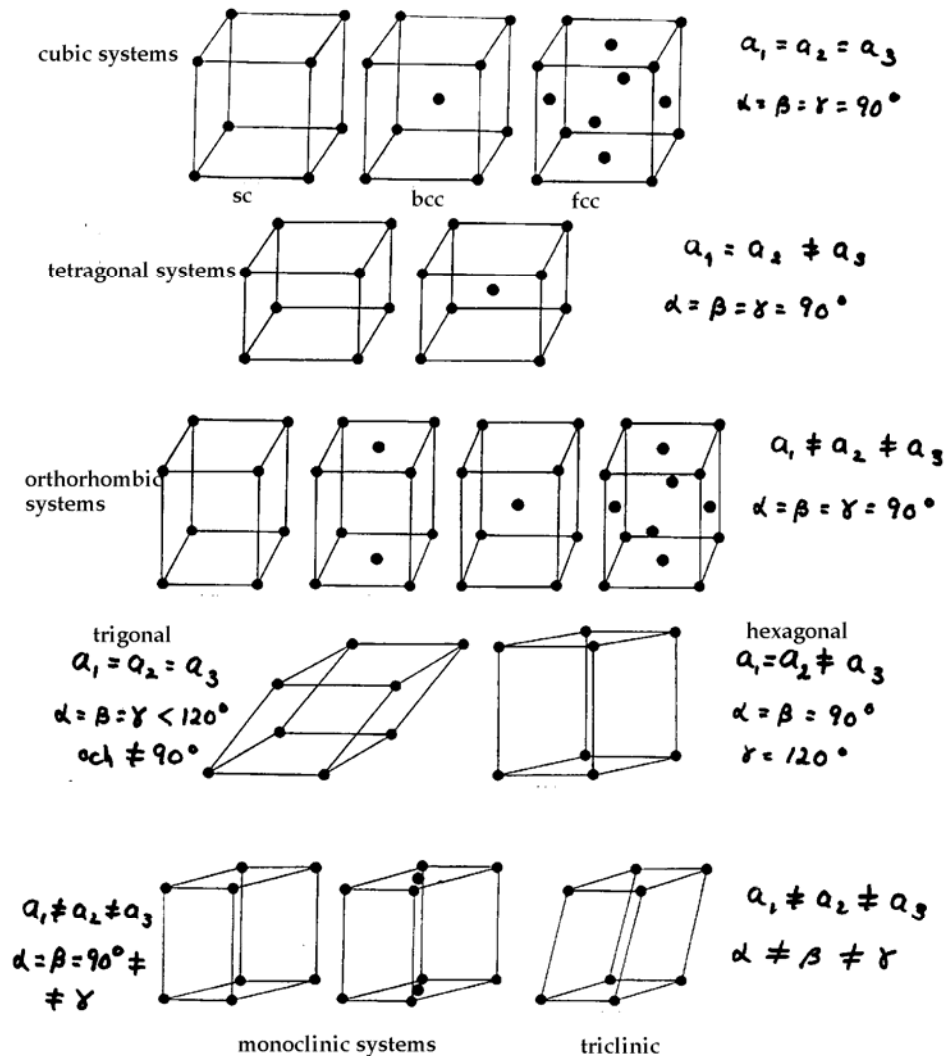

Fig. 1: The 14 Bravais lattices in three dimensions

Considering also the basis, there is a large number of possible crystal structures. The most important additional ones are discussed in K p.13-18. The most common ones among the elements are the body-centered cubic (bcc), face-centered cubic (fcc) and hexagonal close-packed (hcp) ones. The two latter ones are close packed. If we take the atoms to be spheres just touching each other, they will in these structures occupy 74 % of space. The hcp as well as the diamond structures are depicted and discussed by Kittel.

The figures below illustrate the primitive cells, the cubic unit cells and the Wigner-Seitz cells of the bcc and fcc structures. When discussing these structures later in this course we will most often describe them in terms of the cubic crystallographic unit cells.
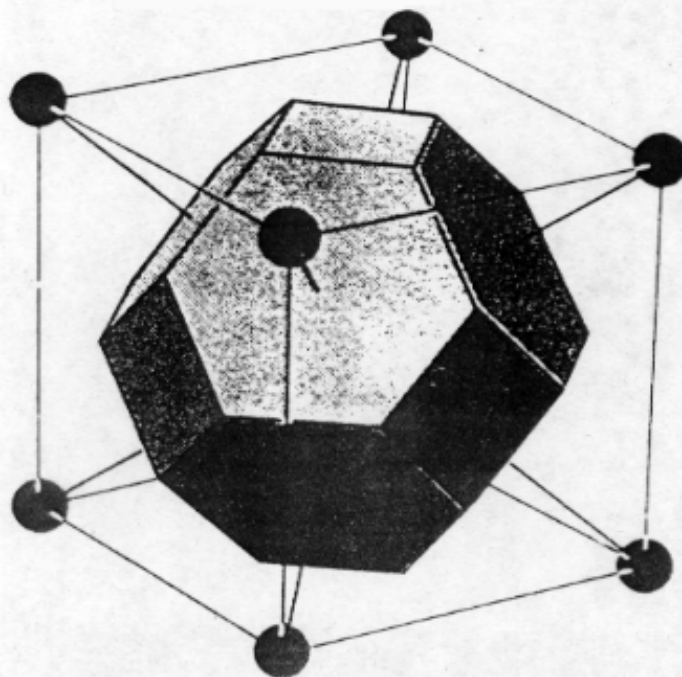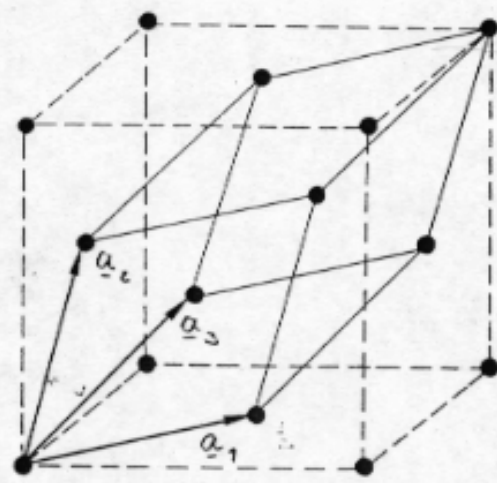
bcc lattice
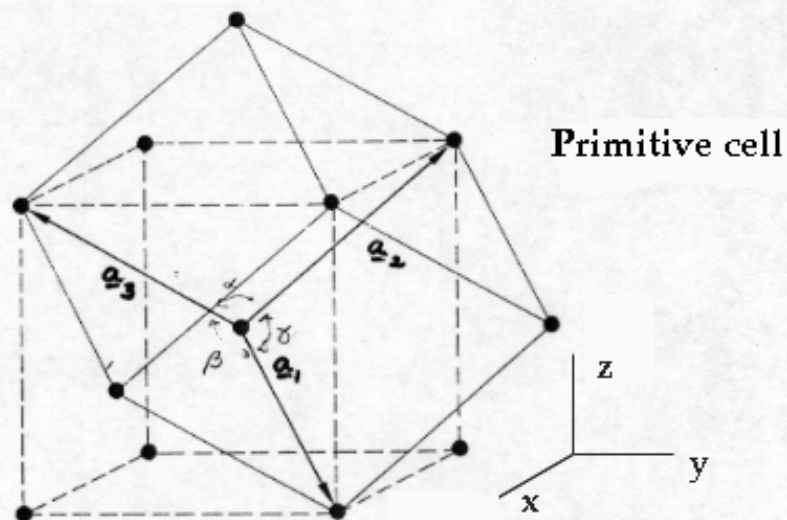
Primitive cell

$$\underline{a}_1 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z}) \qquad \underline{a}_2 = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z})$$

$$\underline{a}_3 = \frac{a}{2}(\hat{x}-\hat{y}+\hat{z})$$ Primitive translation vectors
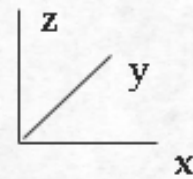
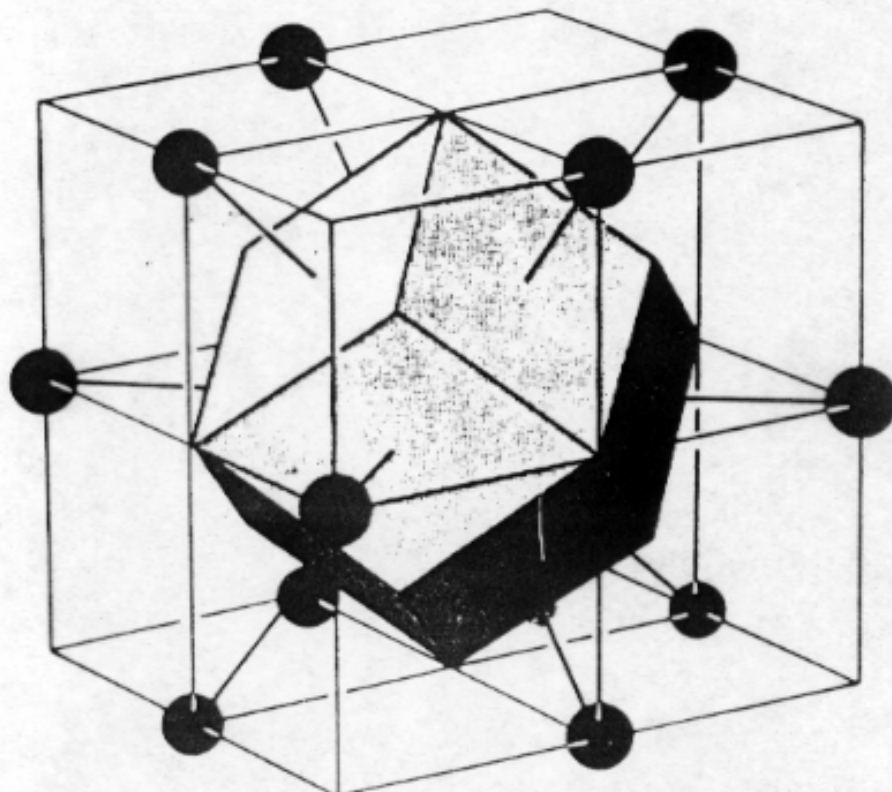**Wigner-Seitz-cell**

fcc lattice

Primitive cell

$$\underline{a}_1 = \frac{a}{2}(\hat{x} + \hat{y}) \qquad \underline{a}_2 = \frac{a}{2}(\hat{y} + \hat{z})$$
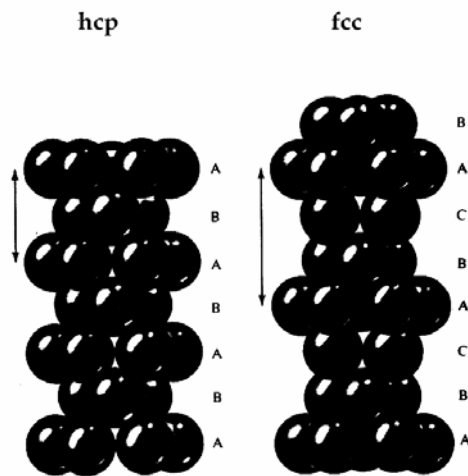
$$\underline{a}_3 = \frac{a}{2}(\hat{z} + \hat{x})$$

Primitive translation vectors

Wigner-Seitz cell

The difference between the close-packed fcc and hcp structures is due to a different way of stacking the close-packed planes (K p. 15). The two different modes of close packing are illustrated in the figure below.

C. Description of Crystal Structures (K p. 11-13).

An alternative description of a lattice is in terms of a set of parallel identical planes. They are defined so that every lattice point belongs to one of these planes. The lattice can actually be described with an infinite number of such sets of planes. This description may seem artificial but we will see later that it is the natural way to interpret diffraction experiments in order to characterize the crystal structure. The figure below shows a 2-D lattice with three different sets of "1-D planes" drawn.

Three families of planes in the lattice

(Miller indices are given)
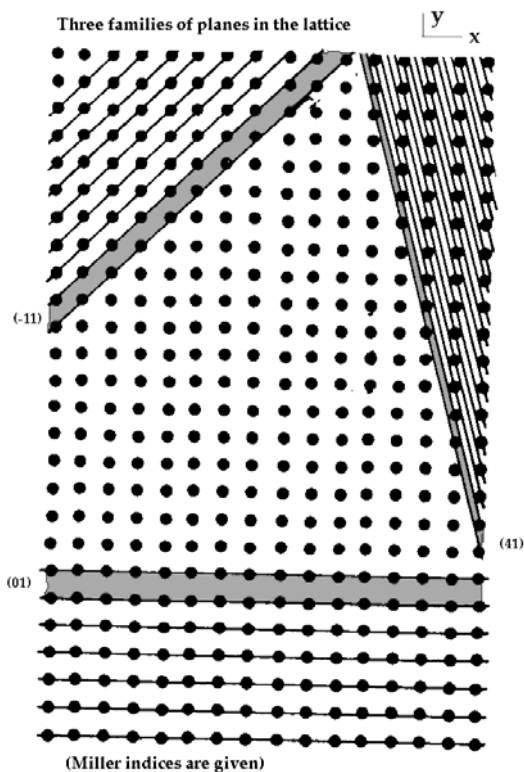
The orientation of a plane can be specified by three integers, the so called **Miller indices**. The intercepts of one plane with the coordinate axes (the fundamental translation vectors of the lattice) are determined and normalized by division by the corresponding lattice constants. Then the reciprocals are taken and reduced to the set of smallest integers. In the figure above, the Miller indices for the three sets of "planes" are given as an example. Note also that the planes in the sets with lower Miller indices are spaced further apart (shaded areas depict the interplanar spacing).

The Miller indices of a single plane or a set of planes are denoted (hkl). All planes with the same symmetry are denoted {hkl}. A direction in a crystal is denoted [uvw] and all equivalent directions (same symmetry) are <uvw>. In cubic crystals [hkl] is orthogonal to (hkl).

In the hcp structure a variation of the index system is often used, the so called **Miller-Bravais indices**. In addition to the primitive translation vectors a_1, a_2 and c, a fourth vector $a_3= - (a_1+a_2)$ is used in order to illustrate the hexagonal symmetry more clearly. The indices are denoted (hkil) with $i=-(h+k)$.

Example: Determine the Miller indices of the set of lines in the two-dimensional case illustrated below. Note that every lattice point will belong to one of the lines in the infinite set.

Construction used to determine Miller indices.