

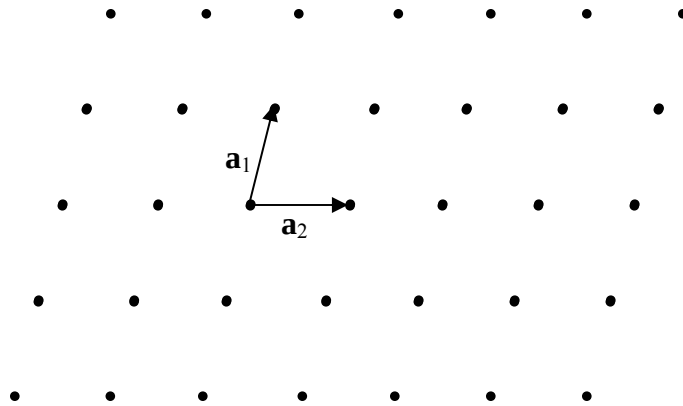
# Chapter 1 Crystal structure

## I. Lattice and basis

1. An ideal crystal is infinite large (hence no boundary surfaces), with identical group of atoms (basis) located at every lattice points in space – no more, no less. In summary:

$$\text{Crystal structure} = \text{Lattice} + \text{basis}$$

2. Lattice points are periodic points in space:



3.  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are the lattice vectors. Every lattice point can be located as

$$\mathbf{r}_{mn} = m \mathbf{a}_1 + n \mathbf{a}_2 \quad (m, n \text{ are integers})$$

or in three dimensional case:

$$\mathbf{r}_{lmn} = l \mathbf{a}_1 + m \mathbf{a}_2 + n \mathbf{a}_3 \quad (l, m, n \text{ are integers})$$

4. Two points,  $\mathbf{r}$  and  $\mathbf{r}'$  related by translational vector

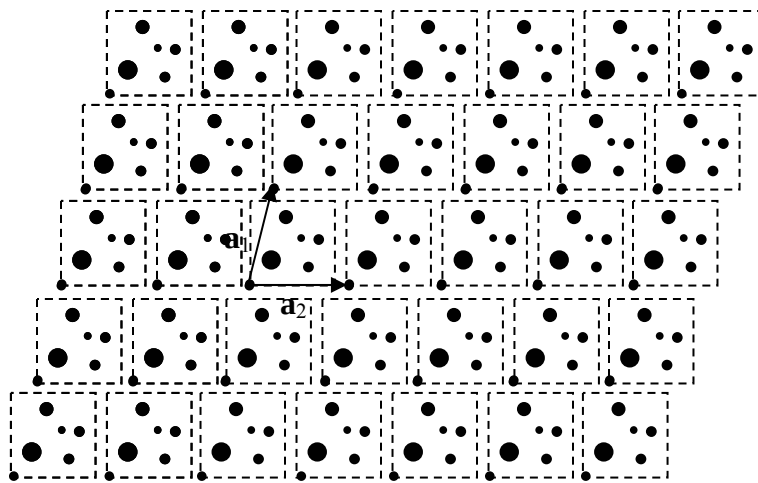
$$\mathbf{r}' = \mathbf{r} + l \mathbf{a}_1 + m \mathbf{a}_2 + n \mathbf{a}_3 \quad (l, m, n \text{ are integers})$$

are equivalent environmentally. Note that  $\mathbf{a}_1, \mathbf{a}_2$ , and  $\mathbf{a}_3$  are lattice vectors and properties of the materials.

5, Congruent groups of atoms locate at each lattice point. This group of atoms is called a basis, e.g.:



6. In this example, the complete crystal structure will look like:



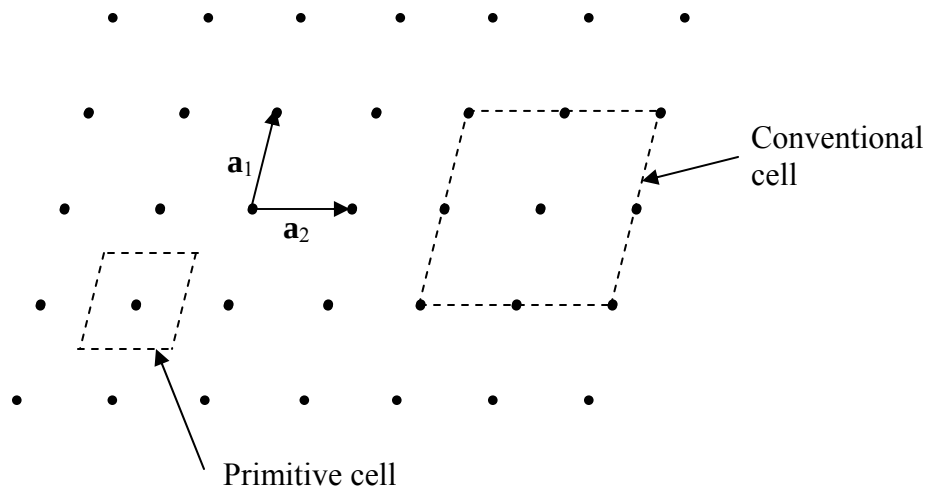
7. Importance of crystal symmetry – Neumann principle: the symmetry elements of any *physical property* must include the symmetry elements of the crystal structure. The physical properties must present a *higher, not lower* symmetry than the crystal structure.

## II. Basis - point groups

1. A basis can possess certain symmetry about the lattice point. These symmetric components are point operation – rotation axis, inversion, mirror (passing through the origin) reflection etc.
2. The symmetry of the basis is specified by the collection of symmetric components forming a group (point group).
3. The point symmetry is restricted because of the translational property of the lattice. The point symmetry should be compatible with that of the lattice. For example, five-fold symmetry is not considered because it is not allowed for the lattice.
4. There are a total of 32 point groups in 3D: 13 single axis + 19 multiple axes = 32 point groups. There are 10 point groups for 2D, and 2 point groups (1 and m) for 1D case.

## III. Lattice – primitive and conventional cells

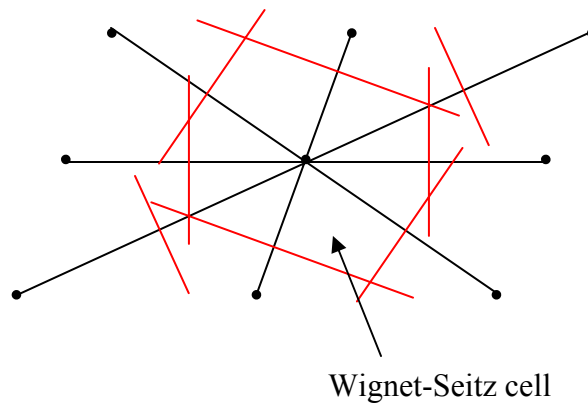
1. A lattice can be formed by repetition (by translation) of a cell.
2. The cell can be either primitive or conventional (non-primitive):



3. The ways to define a primitive cell or conventional cell are not unique.
4. Primitive cell is the most “economic” way to define a cell. There is no overlap if you translate a primitive cell with the lattice vectors. For this reason, all primitive cells have the same volume  $V$ :

$$V = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$$

5. A Wigner-Seitz cell is a primitive cell constructed by the following method:
  - (i) draw lines to connect a given lattice point to all nearby lattice points;
  - (ii) at the mid point and normal to these lines, draw new lines or planes;
  - (iii) the smallest volume enclosed by these new lines or planes is the Wigner-Seitz cell.



6. A non-primitive cell can be considered as a larger primitive cell with a basis.

#### IV. Lattice – 7 crystal system

1. There are 7 lattice configurations possessing different degrees of point symmetry:

|              |                         |                                                     |
|--------------|-------------------------|-----------------------------------------------------|
| Triclinic    | $a_1 \neq a_2 \neq a_3$ | $\alpha \neq \beta \neq \gamma$                     |
| Monoclinic   | $a_1 \neq a_2 \neq a_3$ | $\alpha = \gamma = 90^\circ \neq \beta$             |
| Orthorhombic | $a_1 \neq a_2 \neq a_3$ | $\alpha = \beta = \gamma = 90^\circ$                |
| Tetragonal   | $a_1 = a_2 \neq a_3$    | $\alpha = \beta = \gamma = 90^\circ$                |
| Cubic        | $a_1 = a_2 = a_3$       | $\alpha = \beta = \gamma = 90^\circ$                |
| Trigonal     | $a_1 = a_2 = a_3$       | $\alpha = \beta = \gamma < 120^\circ \neq 90^\circ$ |
| Hexagonal    | $a_1 = a_2 \neq a_3$    | $\alpha = \beta = 90^\circ, \gamma = 120^\circ$     |

These 7 lattice configurations are formed by primitive unit cell

2. The number will expand to 14, called Bravais lattice, if non-primitive cells (or conventional cell) are allowed.

|              |                          |
|--------------|--------------------------|
| Triclinic    | P                        |
| Monoclinic   | P, C                     |
| Orthorhombic | P, C, I, F               |
| Tetragonal   | P, I                     |
| Cubic        | P (sc), I (bcc), F (fcc) |
| Trigonal     | R                        |
| Hexagonal    | P                        |

3. Lattice symbol

| Symbol | Type                    | Positions of additional lattice points      | #lattice points /cell |
|--------|-------------------------|---------------------------------------------|-----------------------|
| P      | primitive               | -                                           | 1                     |
| I      | body centered           | (1/2, 1/2, 1/2)                             | 2                     |
| A      | A-face centered         | (0, 1/2, 1/2)                               | 2                     |
| B      | B-face centered         | (1/2, 0, 1/2)                               | 2                     |
| C      | C-face centered         | (1/2, 1/2, 0)                               | 2                     |
| F      | All faces centered      | (0, 1/2, 1/2), (1/2, 0, 1/2), (1/2, 1/2, 0) | 4                     |
| R      | Rhombohedrally centered | (1/3, 2/3, 2/3), (2/3, 1/3, 1/3)            | 3                     |

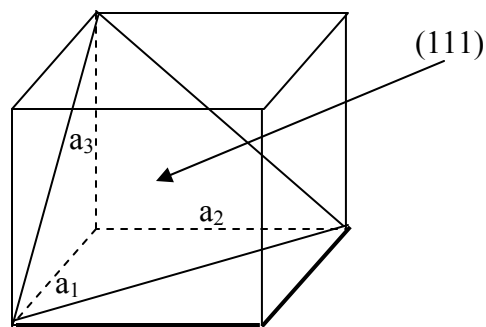
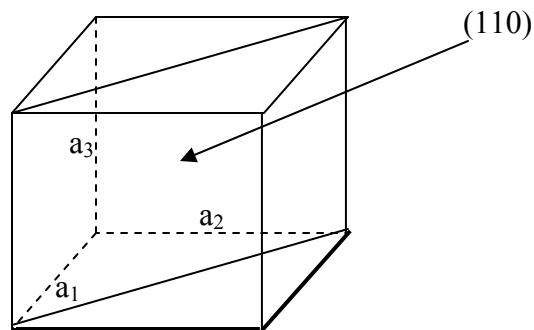
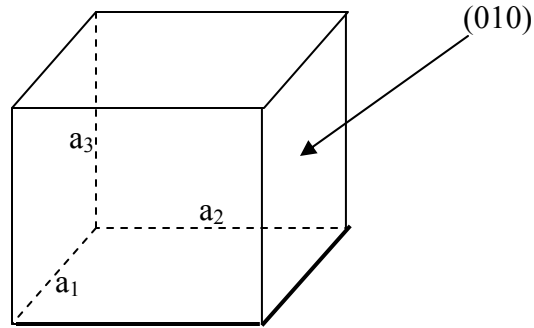
4. When the 32 point groups for the basis are incorporated into the 14 Bravais lattice, there are 230 space groups!

## V. Lattice planes

1. Lattice planes are flat parallel planes separated by equal distance. All the lattice points lie on these lattice planes,
2. Orientation of the lattice planes is specified by the Miller indices (hkl).
3. To determine the Miller indices:

- (i) Find the intercepts on the axes in terms of the lattice constants  $a_1$ ,  $a_2$ ,  $a_3$ .  
The axes may be those of a primitive or nonprimitive cell.
- (ii) Take the reciprocals of these numbers.
- (iii) Reduce the numbers to three smallest integers by multiplying the numbers with the same integral multipliers.
- (iv) The results, enclosed in parenthesis (hkl), are called the Miller indices.

5. Examples:



5. The normal to the plane (hkl) is simply given by the vector  
 $h \mathbf{a}_1 + k \mathbf{a}_2 + l \mathbf{a}_3$

- V. Different types of crystal structure
- 1. Read text (Kittel 8<sup>th</sup> edition p.13-19)