10.3: Lattices and Unit Cells

The regular three-dimensional arrangement of atoms or ions in a crystal is usually described in terms of a space lattice and a unit cell. To see what these two terms mean, let us first consider the two-dimensional patterns shown in Figure 10.3.1. We can think of each of these three structures as a large number of repetitions in two directions of the parallel-sided figure shown immediately below each pattern.

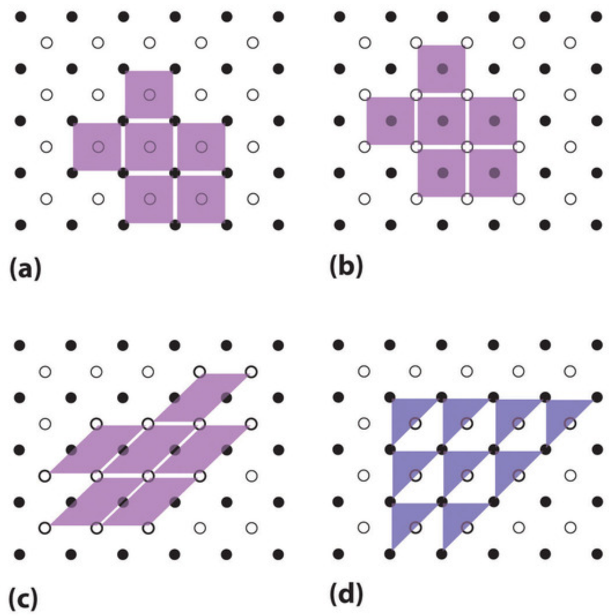

Figure 10.3.1: Unit Cells in Two Dimensions. (a–c) Three two-dimensional lattices illustrate the possible choices of the unit cell. The unit cells differ in their relative locations or orientations within the lattice, but they are all valid choices because repeating them in any direction fills the overall pattern of dots. (d) The triangle is not a valid unit cell because repeating it in space fills only half of the space in the pattern. (CC BY-NC-SA; anonymous by request)

This parallel-sided figure is the **unit cell**. It represents the simplest, smallest shape from which the overall structure can be constructed. The pattern of *points* made by the comers of the unit cells when they are packed together is called the space lattice (Figure 10.3.2). The lines joining the points of the space lattice are shown in color. Without some experience, it is quite easy to pick the wrong unit cell for a given structure. Some incorrect choices are shown immediately below the correct choice in the figure. Note in particular that the unit cell for structure *b*, in which each circle is surrounded by six others at the comers of a hexagon, is *not* a hexagon, but a parallelogram of equal sides (a rhombus) with angles of 60 and 120°.

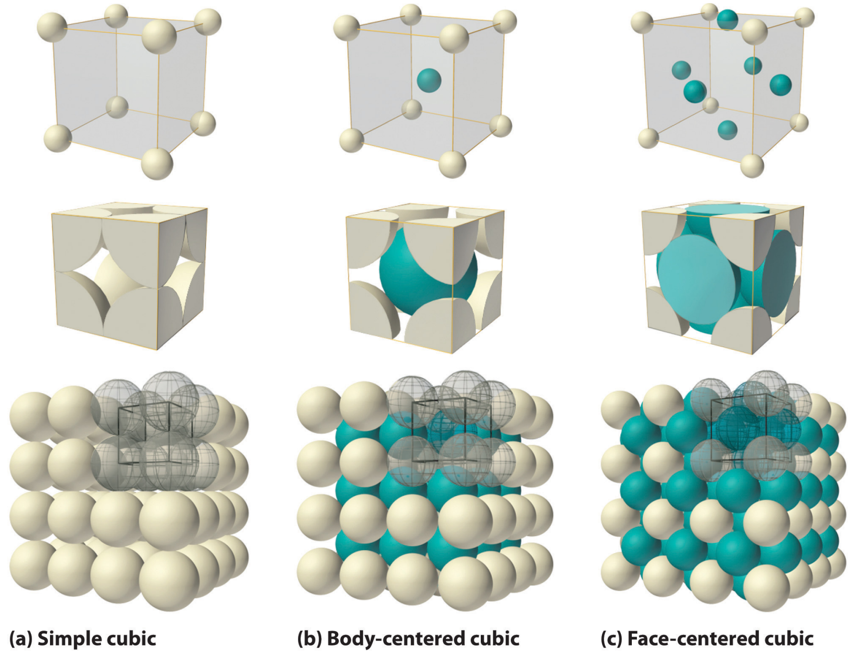

Figure 10.3.2: The Three Kinds of Cubic Unit Cell. For the three kinds of cubic unit cells, simple cubic (a), body-centered cubic (b), and face-centered cubic (c), there are three representations for each: a ball-and-stick model, a space-filling cutaway model that shows the portion of each atom that lies within the unit cell, and an aggregate of several unit cells. (CC BY-NC-SA; anonymous by request)

Figure 10.3.2 illustrates the space lattice and the unit cell for a real three-dimensional crystal structure—that of sodium chloride.

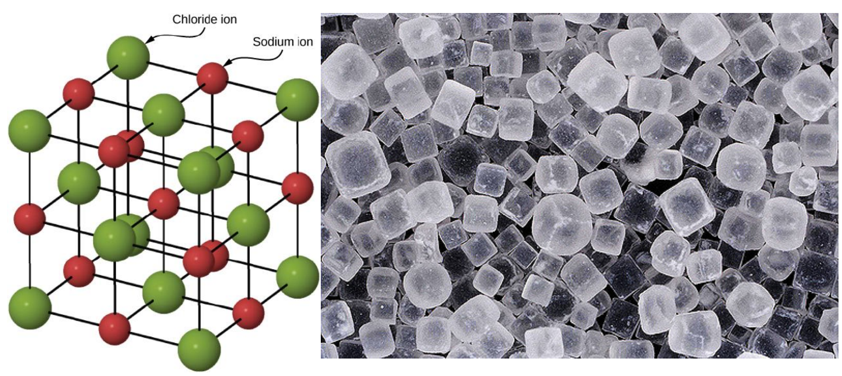

Figure 10.3.3: (left) The crystal lattice and unit cell of a crystal of sodium chloride. Structure of the sodium chloride crystal. The sodium and chloride ions are around in a face-centered cubic (FCC) structure. Sodium ions, Na^+, are shown in red. Chloride ions, $Cl^–$, are shown in green. (right) The macroscopic image on the right shows salt cubes, which demonstrate the cubic unit cell of NaCl (it doesn't always turn out this way, since crystal growth is a complex process its not guaranteed that the macroscopic crystal structure matches the unit cell). (CC BY; OpenStax)

This is the same structure that was shown for lithium hydride, except that the sizes of the ions are different. A unit cell for this structure is a cube whose comers are all occupied by sodium ions. Alternatively, the unit cell could be chosen with chloride ions at the comers.

The unit cell of sodium chloride contains *four* sodium ions and *four* chloride ions. In arriving at such an answer we must bear in mind that many of the ions are shared by several adjacent cells (part *c* of Figure 10.3.2 shows this well). Specifically, the sodium ions at the centers of the square faces of the cell are shared by two cells, so that only half of each lies within the unit cell. Since there are six faces to a cube, this makes a total of three sodium ions. In the middle of each edge of the unit cell is a chloride ion which is shared by four adjacent cells and so counts one-quarter. Since there are twelve edges, this makes three chloride ions. At each comer of the cube, a sodium ion is shared by eight other cells. Since there are eight comers, this totals to one more sodium ion. Finally, there is a chloride ion in the body of the cube unshared by any other cell. The grand total is thus four sodium and four chloride ions.

A general formula can be derived from the arguments just presented for counting *N*, the number of atoms or ions in a unit cell. It is:

$$N = N_{\text{body}} + \frac{N_{\text{face}}}{2} + \frac{N_{\text{edge}}}{4} + \frac{N_{\text{corner}}}{8}$$