

Introduction

We often think of crystals as the gemstones we give to a loved one, but most metals (e.g. copper, aluminum, iron) that we encounter daily are common crystals too. In this chapter, we will examine the structure of crystalline matter in which particles are arranged in a repeating pattern that extends over very long distances. This long-range order is formally described by identifying small local groupings of particles, known as a *basis* set, that are identically affixed to the sites of a regularly repeating space *lattice*. As it happens, most crystals found in nature assume one of a limited set of special space lattices known as Bravais lattices. These lattices are special by virtue of their unique symmetry properties wherein only discrete translations and rotations allow the lattice to appear unchanged. Chief among these Bravais lattices are the cubic and hexagonal lattice structures that appear most frequently in nature. We focus extra attention on both to provide a useful introduction to coordination properties and packing fractions.

1.1 Crystal lattice

Crystals have a decided advantage because of the inherent repeating pattern present in their structure. In an ideal (perfect) crystal, this repeating pattern extends indefinitely. However, for real crystals found in nature, the pattern is often interrupted by imperfections known as *defects* that can include vacancies, in which a single particle is missing, and dislocations in which the repeating pattern is offset. These defects are important for some crystal properties, but for now we restrict ourselves to only ideal structures. Besides, even in real crystals large regions containing substantial numbers of particles exist in which a perfectly repeating pattern is maintained.

Let's start with an imaginary, two-dimensional example of a crystal that contains two types of particles (say, large A atoms and small B atoms) as illustrated in Fig. 1.1. It is clear from inspection that this collection of particles displays a well-ordered repeating pattern of A and B atoms that can be

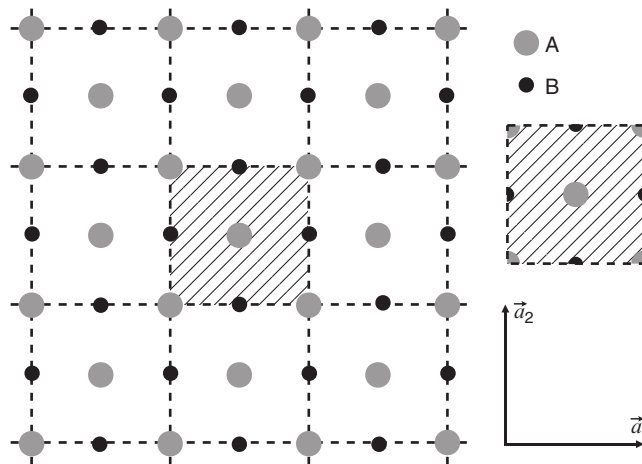


Figure 1.1

The repeating pattern of atoms A (gray circles) and B (black circles) is mapped onto a lattice (dashed lines) that is defined by two lattice vectors (\vec{a}_1 and \vec{a}_2). The pattern of atoms can be viewed as the result of attaching tiles (hashed area that contains a total of two A atoms and two B atoms) onto the lattice.

arranged neatly on the square grid that is superimposed. How can we best describe this repeating pattern? We could simply establish an arbitrary origin and then list the position vectors for every particle of each type. But that would be unnecessarily cumbersome given that there is an obvious repeating pattern. Instead, consider the square grid. The points formed by the intersections of these grid lines can be referenced from any other point by any combination of translations of the form:

$$\vec{T} = h\vec{a}_1 + k\vec{a}_2, \quad (1.1)$$

where h and k are the complete set of integer numbers. The complete set of these translations define what is known as a *space lattice* – an abstract set of points in space that convey the inherent repeating pattern behind the crystal's structure.

In Fig. 1.1, we see that some of the larger A atoms are located directly on the points of the space lattice (grid) and their positions can be referenced by the set of translations in Eq. (1.1) alone. But other A atoms, as well as the smaller B atoms, reside off the lattice. To completely describe the particle positions of all the atoms of the crystal, we must combine with the space lattice a small subset of atoms (known as a *basis*) that are repeatedly attached to each lattice site so as to produce the entire structure. This is much like flooring your kitchen with linoleum tiles. Imagine that each linoleum tile has a pattern stamped onto it corresponding to one of the squares in Fig. 1.1. This particular tile would have two of each type of atom: a complete A atom at the center, one-quarter of an A atom at each corner, and one-half of a B atom at the middle of

each side. When each such tile is positioned with its lower left-hand corner coincident with a space lattice point, the completed assembly of tiles would reproduce the crystal structure of Fig. 1.1 as a whole.

1.1.1 Basis set

Thus, to describe the entire structure of a crystal we combine a space lattice, described by the translations of Eq. (1.1), with a set of basis vectors (referenced to, say, the lower left-hand corner of the tile) to describe the contents of each tile:

$$\vec{R}_i = x_i \vec{a}_1 + y_i \vec{a}_2, \quad (1.2)$$

where x_i and y_i are fractions. For the particular tile illustrated in Fig. 1.1, the basis vectors would include:

$$\begin{aligned} \text{single central A atom: } & \vec{R}_1 = \frac{1}{2} \vec{a}_1 + \frac{1}{2} \vec{a}_2 \\ \text{four corner A atoms: } & \left. \begin{aligned} \vec{R}_2 &= 0 \vec{a}_1 + 0 \vec{a}_2 \\ \vec{R}_3 &= 1 \vec{a}_1 + 0 \vec{a}_2 \\ \vec{R}_4 &= 0 \vec{a}_1 + 1 \vec{a}_2 \\ \vec{R}_5 &= 1 \vec{a}_1 + 1 \vec{a}_2 \end{aligned} \right\} \frac{1}{4} \text{ of an A atom each} \\ \text{four side B atoms: } & \left. \begin{aligned} \vec{R}_6 &= \frac{1}{2} \vec{a}_1 + 0 \vec{a}_2 \\ \vec{R}_7 &= 0 \vec{a}_1 + \frac{1}{2} \vec{a}_2 \\ \vec{R}_8 &= 1 \vec{a}_1 + \frac{1}{2} \vec{a}_2 \\ \vec{R}_9 &= \frac{1}{2} \vec{a}_1 + 1 \vec{a}_2 \end{aligned} \right\} \frac{1}{2} \text{ of a B atom each} \end{aligned}$$

This is still more cumbersome than necessary. Consider, as shown in Fig. 1.2, an alternative space lattice composed of diagonal grid lines. Notice that we

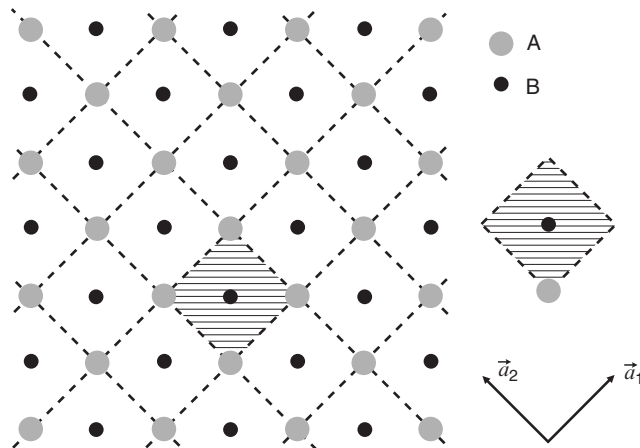


Figure 1.2

The same pattern of two atoms found in Fig. 1.1 are referenced to an alternative, diagonal lattice with a corresponding redefinition of the tile (hashed area) to contain only one each of each atom.

have not repositioned any of the particles, only redefined the space lattice we choose to associate with them. Our diamond-shaped tiles now contain only one atom of each type. This sort of tile is known as a *primitive cell*. It is the smallest-sized tile that can be used together with the space lattice to fill the space with our desired repeating pattern. Our basis set now requires only two vectors:

$$\begin{aligned} \text{A atom: } \vec{R}_1 &= 0\vec{a}_1 + 0\vec{a}_2 \\ \text{B atom: } \vec{R}_2 &= \frac{1}{2}\vec{a}_1 + \frac{1}{2}\vec{a}_2. \end{aligned} \quad (1.3)$$

Note here that the entire A atom is now being associated with the tile (even though three quarters of it sticks outside). Tiles affixed to neighboring lattice sites will then provide the other three A atoms.

1.1.2 Primitive cells

Primitive cells can be identified by several properties. A primitive cell:

- (1) contains only one lattice point,
- (2) has the smallest size (area, $A = |\vec{a}_1 \times \vec{a}_2|$) that can just fill the space by repetition, and
- (3) has a basis set containing only one molecular unit (in our case: AB).

Primitive cells are *not* unique. As shown in Fig. 1.3, yet another alternative space lattice has been chosen to describe our AB system. The shaded cell shown has the same smallest size area as our diamonds in Fig. 1.2 and contains

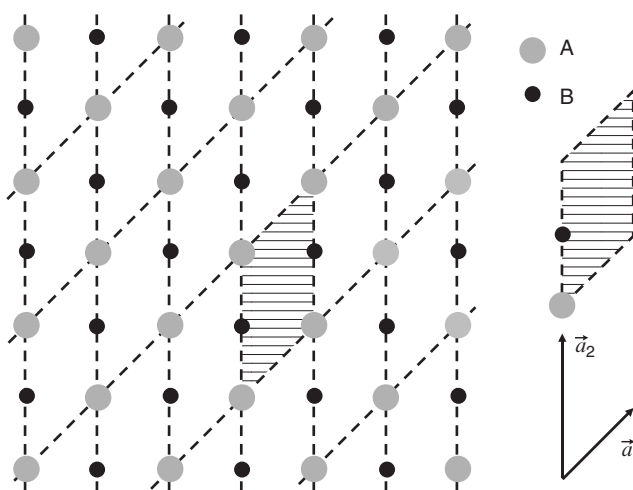


Figure 1.3

The same pattern of two atoms found in Fig. 1.1 and Fig. 1.2 are referenced to yet another alternative lattice with an alternative primitive cell (hashed area).

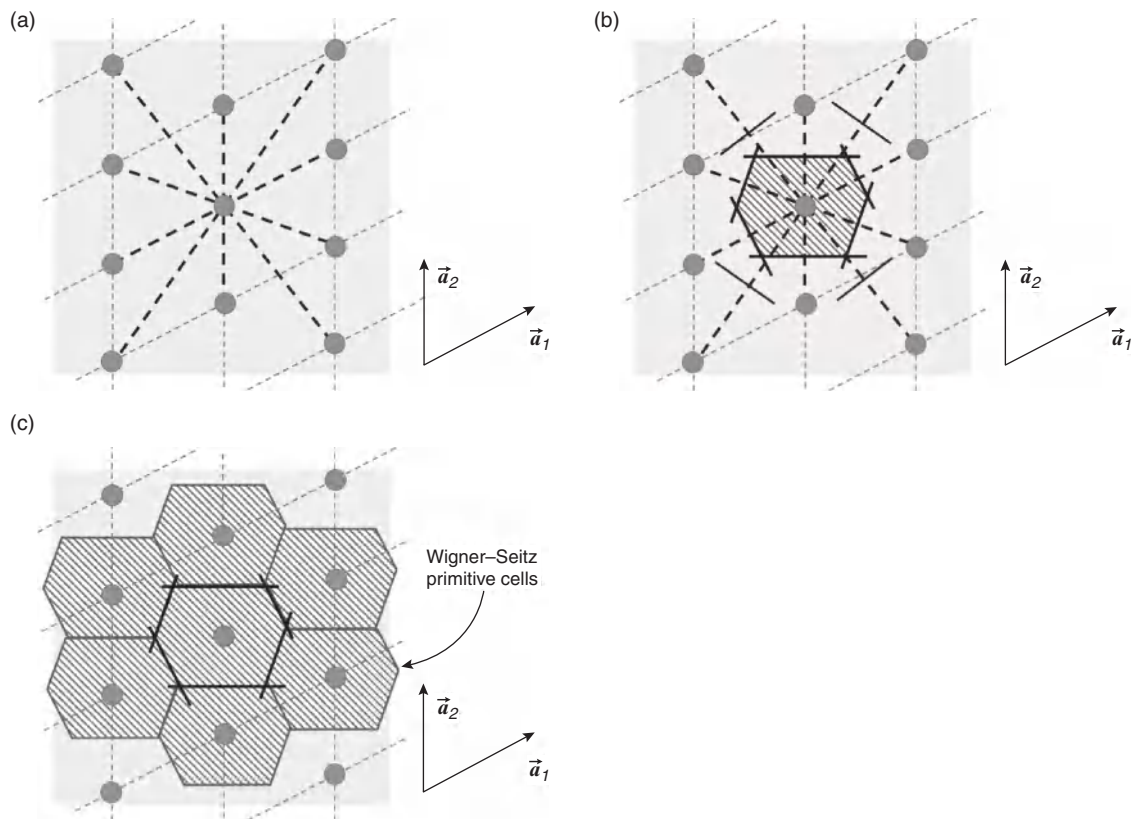


Figure 1.4

Steps in construction of the Wigner–Seitz primitive cell. (a) Lines are first drawn from a central lattice site to all neighboring sites (heavy dashed lines). (b) Each of these lines is then bisected by a perpendicular plane (heavy solid lines) and the volume enclosed becomes the Wigner–Seitz cell. (c) The cell is capable of tiling the entire space and is a primitive cell because it contains one lattice site (at its center).

one of each atom type. However, the basis vectors for this situation would need to be revised as:

$$\begin{aligned} \text{A atom: } \vec{R}_1 &= 0\vec{a}_1 + 0\vec{a}_2 \\ \text{B atom: } \vec{R}_2 &= 0\vec{a}_1 + \frac{1}{2}\vec{a}_2. \end{aligned} \quad (1.4)$$

Wigner–Seitz primitive cell

Although there are many choices for the primitive cell as illustrated above, there is one alternative known as the *Wigner–Seitz cell*, which will have special relevance later on in our discussions of solid state physics. Construction of the Wigner–Seitz cell is illustrated in a series of panels in Fig. 1.4 and begins

by drawing lines from any arbitrary lattice site to neighboring lattice sites (see Fig. 1.4a). Next, each line is bisected by a perpendicular line (or plane in the case of a 3D lattice), as illustrated in Fig. 1.4b. The interior region bounded by these perpendicular lines is then the Wigner–Seitz cell. The cell is seen to be primitive because it contains just one lattice point (namely, the one at its center) and can successfully tile the entire space.

1.2 Symmetry

Aside from its repeating pattern, the space lattice possesses another important characteristic known as *symmetry*. Consider yourself as a (very small) observer located on one of the A atoms in Fig. 1.5. When you look around, you observe nearby B atoms (to the north, south, east and west) and nearby A atoms (to the NE, NW, SE and SW). If you now move to another point of the space lattice (atop another A atom), by a translation, $\vec{T} = h\vec{a}_1 + k\vec{a}_2$, you will experience no sense that your surroundings have changed in any way. In this way the space lattice is said to possess *translational symmetry* – if the entire space lattice is shifted by any of the translation vectors that describe it, the resulting pattern is unchanged in any observable manner.

In addition to this translational symmetry, which all space lattices possess by virtue of their repeating nature, there are other important symmetry operations that define different space lattices. For example, consider yourself again atop an A atom in Fig. 1.5. If you rotate by 90° you again see the same surroundings as before you rotated. The space lattice is said to possess a certain *rotational symmetry*. Note that this symmetry appears only for specific angles of rotation in

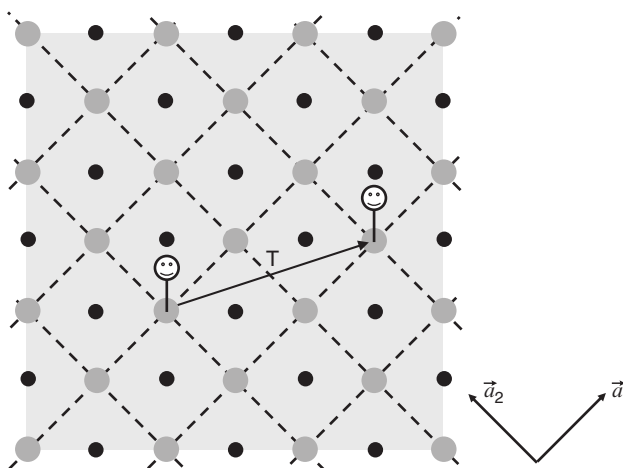


Figure 1.5

An observer situated on a lattice undergoes a translation to any other lattice site and finds his/her surroundings unaltered. The system of particles is then said to possess translational symmetry.

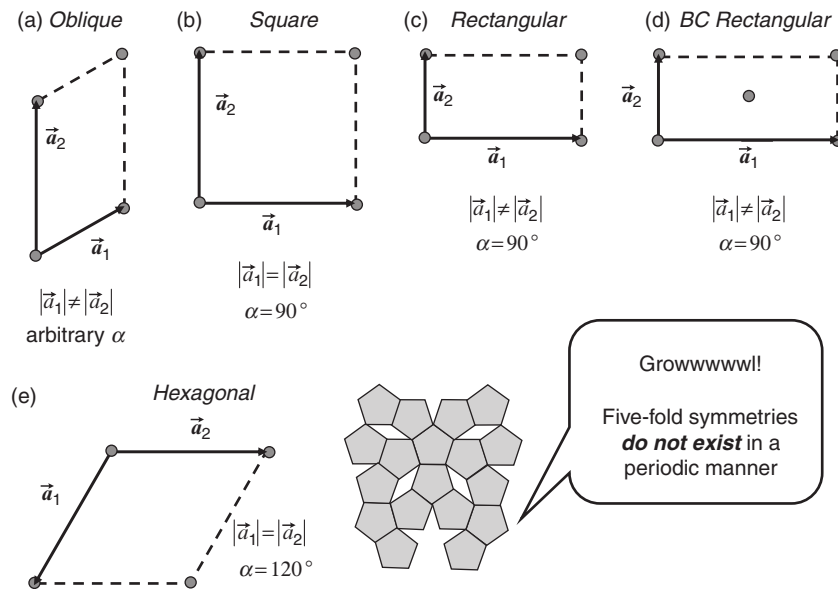


Figure 1.6

The complete set of Bravais lattices (nets) in two dimensions. In addition to the oblique, there are four other lattices possessing distinct symmetry properties. Of these, only the BC rectangular is a conventional lattice. Rotational symmetries include 2, 3 and 4-fold but do not allow for 5-fold symmetries.

the crystal. For example, a rotation by 45° on the lattice of Fig. 1.5 will not return your surroundings to their original state. Only rotations by a multiple of 90° will do this. Because there are four 90° increments in a full circle, this particular case of rotational symmetry is referred to as ‘4-fold’ rotational symmetry.

For the two-dimensional situations we are currently discussing, there are an unlimited number of possible space lattices owing to the fact that any lengths of the two lattice vectors (\vec{a}_1 and \vec{a}_2) can be chosen as well as any angle between them. However, these generic, *oblique* lattices like that shown in Fig. 1.6a will only have 2-fold rotational symmetry unless special restrictions are applied to the lattice vectors. Special lattices, known as *Bravais lattices*, can be obtained with higher degrees of rotational symmetry by placing restrictions on the lengths and angles between the two lattice vectors \vec{a}_1 and \vec{a}_2 . For 2D, there are just four other lattices that can be constructed with other than 2-fold symmetry. These are shown in Fig. 1.6. Note that 5-fold symmetry is not possible. As one can see in Fig. 1.6, primitive cells based on pentagons do not correctly fill space.

Additional symmetry operations under which certain space lattices will return to their original situation include:

- (1) Mirror symmetry: reflection about a plane.
- (2) Inversion symmetry: rotation by 180° about an axis followed by reflection through a plane normal to the rotation axis.

- (3) Glide symmetry: a combination of reflection and translation.
- (4) Screw symmetry: a combination of rotation and translation.

1.2.1 Conventional cells

One of the lattices presented in Fig. 1.6 is not a primitive lattice. The lattice shown in Fig. 1.6d has lattice vectors identical with those in Fig. 1.6c, but has an additional lattice point at the center of the cell. In this instance, the two lattice vectors mark off a *conventional unit cell* (non-primitive) referred to as a ‘body-centered’ (BC) rectangular lattice. Conventional cells are often introduced as an alternative to their primitive lattices as they afford a better visualization of the geometrical structure.

1.3 Bravais lattices

Our discussion of 2D lattices has laid much of the groundwork for discussing lattices in three dimensions. The structures of 3D crystals are again defined by the combination of a space lattice, described by a set of translation vectors:

$$\vec{T} = h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3, \quad (1.5)$$

where h , k and l are the complete set of integers, and an appropriate set of basis vectors:

$$\vec{R}_i = x_i\vec{a}_1 + y_i\vec{a}_2 + z_i\vec{a}_3, \quad (1.6)$$

that locate the contents of each unit cell in relation to any given lattice point. The volume of a 3D cell is now given by

$$V = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| \quad (1.7)$$

and is smallest for any of the possible primitive cells that can be constructed.

While any sort of generic lattice could be created with appropriate choice of the lengths of the three lattice vectors (\vec{a}_1 , \vec{a}_2 and \vec{a}_3) as well as the angle between them, symmetry considerations lead to only 13 other, special or *Bravais lattices*. All 14 lattice types are illustrated in Fig. 1.7. The generic lattice (with arbitrary lengths and angles between \vec{a}_1 , \vec{a}_2 and \vec{a}_3) is known as the triclinic, and the other 13 are grouped into six sub-categories based on how the lattice vectors are restricted to produce a unique symmetry: monoclinic, orthorhombic, tetragonal, cubic, trigonal and hexagonal. In addition to the primitive cell forms, some of these categories also contain conventional cell forms. These are non-primitive cells in which more than one lattice point is included in the cell. As the majority of crystals found in nature assume either a cubic or a hexagonal lattice structure, we focus next on the detailed properties of these two lattice types.

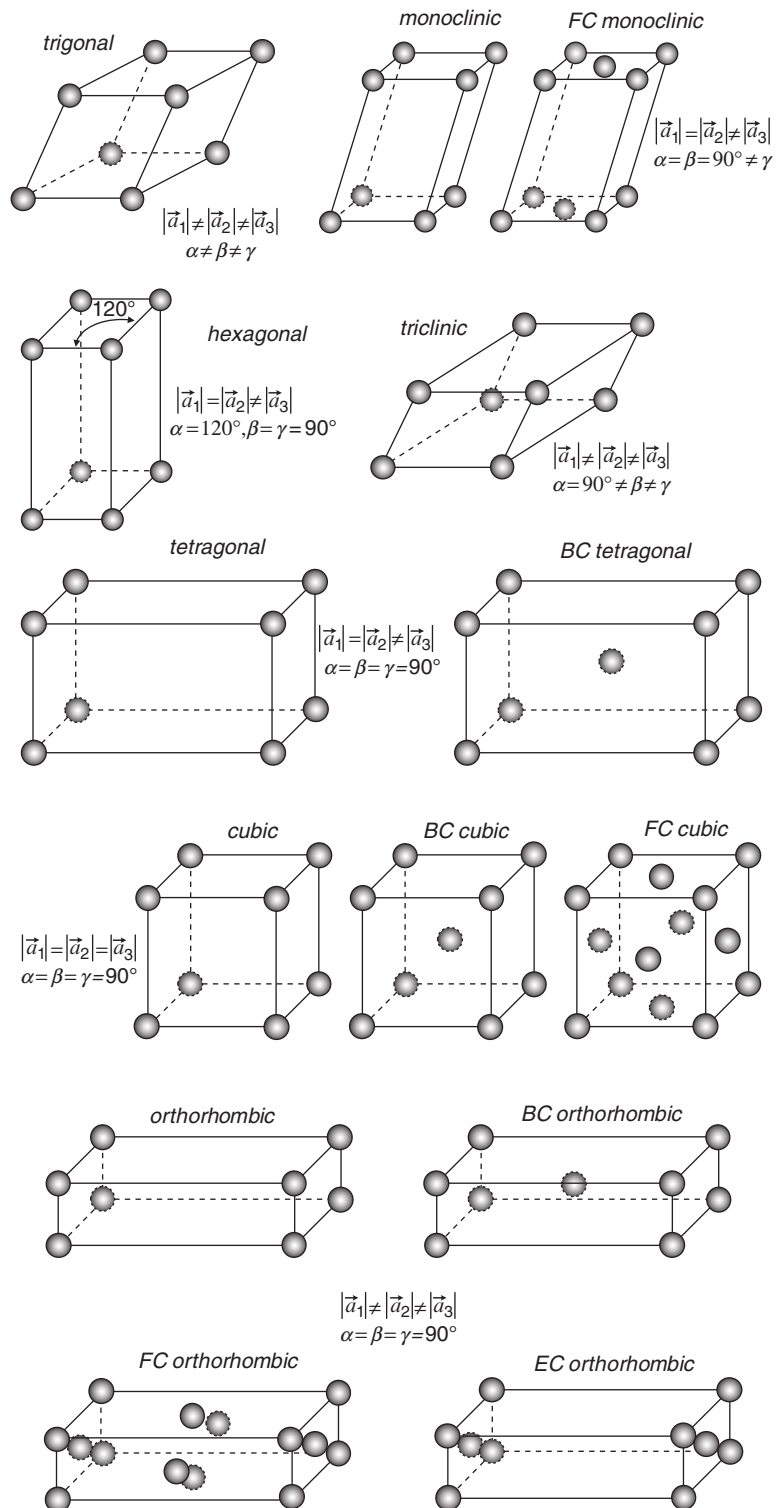


Figure 1.7

The complete set of 14 Bravais lattices in three dimensions grouped into seven sets: trigonal, monoclinic, hexagonal, triclinic, tetragonal, cubic and orthorhombic.

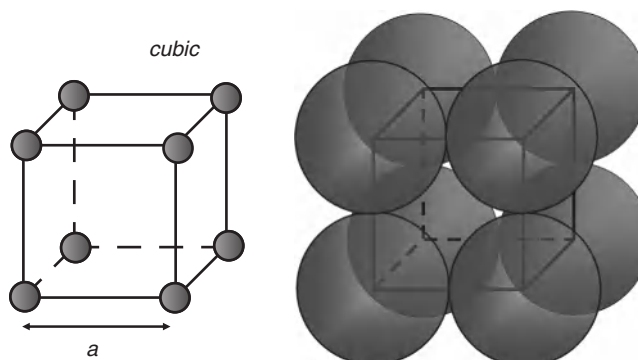


Figure 1.8

The simple cubic lattice. The ideal packing fraction is determined by imagining that balloons at each lattice site are inflated to just touch one another, as shown in the right-hand figure.

1.3.1 Cubic lattices

The cell of a simple cubic (SC) lattice, shown in Fig. 1.8, is a primitive cell because it contains just one lattice site. To see this, you may need to pretend that the lattice points in each corner of the cube are actually finite-sized balls. One-eighth of a ball at each corner resides inside the cube while the remaining seven-eighths resides in other adjacent cells. Thus, in spite of it having eight corners, any given cell contains just one total lattice site. Because the lengths of the three lattice vectors are equivalent and orthogonal, the cell volume is simply $V = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3| = a^3$.

This simple cubic structure is to be contrasted with the two conventional cell structures of the body-centered cubic (BCC) and face-centered cubic (FCC) types. The body-centered cubic (BCC) has *two* lattice points per cell (one in the center and one-eighth in each of eight corners) and the face-centered cubic (FCC) has *four* lattice points per cell (one-eighth in each of the corners and one-half in each of six faces). While the FCC and BCC cells are conventional, each can alternatively be described by corresponding primitive cells affixed to a non-cubic lattice. Since a primitive cell must contain only one lattice point, a direct way of constructing these primitive cells would be to assign an origin to any one of the lattice sites, and choose lattice vectors (\vec{a}'_1 , \vec{a}'_2 and \vec{a}'_3) that correspond to the shortest distance to three neighboring lattice sites which are oriented so as to trace out a rhombohedral with the minimum volume. The result is shown in Fig. 1.9 for both situations. With a little effort, one can show (Ex. 1 and Ex. 2) that the volumes of these two primitive cells are $a^3/2$ for the BCC and $a^3/4$ for the FCC, as expected.

Packing fractions

Another important property of any structural arrangement of particles is the *packing fraction*. The ideal packing fraction is a measure of how much space is

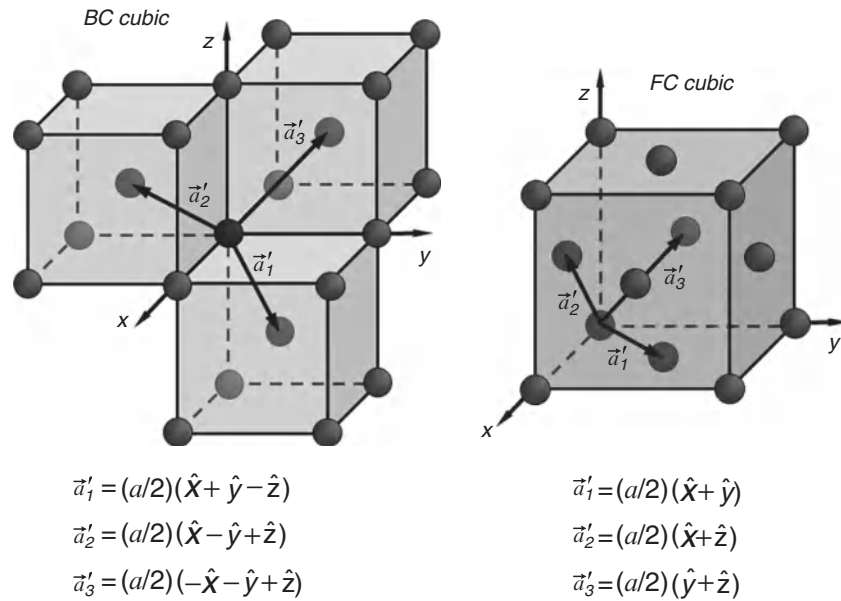


Figure 1.9

Lattice vectors for the corresponding primitive lattice of both the BC cubic and FC cubic conventional lattices.

occupied by identical spherical atoms when they are placed on the lattice sites such that they just touch one another. Imagine that inflatable balloons are located at the corners of the cube in Fig. 1.8 and are inflated at equal rates until they just begin to touch. Each balloon will have a radius equal to half the lattice spacing ($a/2$) and one-eighth of its volume will reside inside the cube. Hence the total space inside the cube that is physically occupied by the inflated balloons is $4\pi(a/2)^3/3 = 0.524a^3$, and the fraction of *occupied* space (the packing fraction) would be 0.524. A similar analysis (Ex. 3 and Ex. 4) of the BCC and FCC lattices, results in packing fractions of 0.680 and 0.740, respectively. These higher packing fractions are to be anticipated since, in each case, the BCC and FCC structures represent an attempt to compensate for the empty space of the SC lattice, which is seen in Fig. 1.8 to be concentrated in the cube center and at the center of each face.

Coordination spheres

Yet another characteristic of lattice structure is its coordination properties. This concerns the number of nearest (or next-nearest) neighboring lattice points and their distance. Consider again the SC lattice in Fig. 1.8. For a given lattice point, the shortest distance to another lattice site is the lattice spacing a . If we search around any given lattice point at this distance we will encounter six other lattice sites. Hence, the nearest neighbor *coordination number* for the SC

Table 1.1 Properties of cubic lattices.			
	SC	BCC	FCC
Conventional cell volume	a^3	a^3	a^3
Lattice points per cell	1	2	4
Primitive cell volume	a^3	$a^3/2$	$a^3/4$
Nearest neighbors	6	8	12
Nearest neighbor separation	a	$\sqrt{3}a/2$	$a/\sqrt{2}$
Next-nearest neighbors	12	6	6
Next-nearest neighbor separation	$\sqrt{2}a$	a	a
Packing fraction	$\pi/6 = 0.524$	$\sqrt{3}\pi/8 = 0.680$	$\sqrt{2}\pi/6 = 0.740$

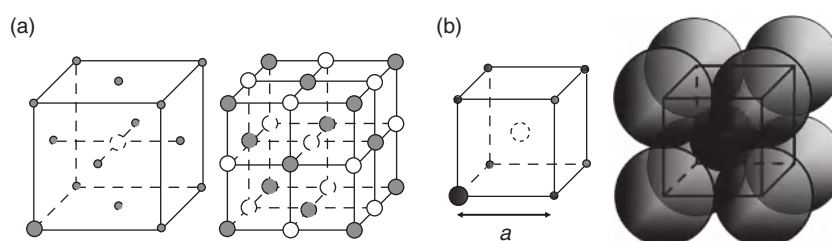


Figure 1.10

(a) The FC cubic structure of NaCl. Left-hand figure highlights the diatomic basis set consisting of one Cl anion (large solid circle) and one Na cation (large open circle in cube center). Right-hand figure shows the result when this basis set is attached to the sites of a FC cubic lattice.

(b) The simple cubic structure of CsCl. Left-hand figure highlights the diatomic basis set consisting of one Cl anion (large solid circle) and one Cs cation (large open circle in cube center). Right-hand figure illustrates how the smaller size of the Cs cation is comfortably fitted to the void space present in the SC center.

lattice is six. Likewise, the next largest distance to another lattice site is $\sqrt{2}a$ and we will find a *next-nearest* neighbor coordination number of 12. A summary of the coordination properties and ideal packing fractions of cubic lattices is provided in Table 1.1.

Rocksalt and diamond

Now let's consider some common examples of cubic crystals found in nature to see how their lattice structures arise. First we consider NaCl (rocksalt) whose Na^+ and Cl^- atoms are arranged as shown in Fig. 1.10a. The structure is built from a FCC space lattice containing a basis of two atoms:

$$\begin{aligned} \text{Cl atom: } \vec{R}_{Cl} &= 0\vec{a}_1 + 0\vec{a}_2 + 0\vec{a}_3 \\ \text{Na atom: } \vec{R}_{Na} &= \frac{1}{2}\vec{a}_1 + \frac{1}{2}\vec{a}_2 + \frac{1}{2}\vec{a}_3. \end{aligned} \quad (1.8)$$

Because the FCC conventional cell contains four lattice points, we should find four units of the chemical formula (NaCl) present in each cell. Let's check. Each one of eight corners provides one-eighth of a Cl anion and each one of six faces provides one-half of a Cl anion inside the cell, resulting in a total of four Cl anions per cell. Likewise, there is one entire Na cation in the cell center and each of 12 edges provide one-quarter of a Na cation, resulting in a total of four Na cations per cell.

Compare this NaCl structure with that of a chemically equivalent salt, CsCl, shown in Fig. 1.10b. Interestingly enough, the structure here is *not* built on the FCC lattice, but on the SC lattice with a basis of two atoms:

$$\begin{aligned} \text{Cl atom: } \vec{R}_{Cl} &= 0\vec{a}_1 + 0\vec{a}_2 + 0\vec{a}_3 \\ \text{Cs atom: } \vec{R}_{Cs} &= \frac{1}{2}\vec{a}_1 + \frac{1}{2}\vec{a}_2 + \frac{1}{2}\vec{a}_3. \end{aligned} \quad (1.9)$$

Because the SC is a primitive cell, it should contain just one unit of the chemical formula CsCl, and indeed it does. Why though does CsCl not assume the FCC structure like NaCl? This difference stems from the differing sizes of the ions and an inherent tendency for nature to favor efficient packing of space. In NaCl, the Na^+ and Cl^- are nearly equal in diameter and, in this instance, space is best filled by using the FCC structure. However, Cs^+ is much smaller in diameter and space is more efficiently occupied using the SC lattice. Thus the crystalline structure realized in nature is a consequence of many factors including the size of the particles, their bonding requirements, and a desire to minimize empty space.

As another example, we consider the structure of diamond. Diamond is composed entirely of C atoms that are bonded covalently. Because of the discrete nature of the covalent bond, each C atom must form a single covalent bond with four other C atoms in order to satisfy the requirement of a closed electronic shell configuration. This bonding requirement promotes a *tetragonal* aspect of the diamond structure, which can be seen in Fig. 1.11a. Here the diamond structure is composed of an FCC lattice with a basis of two identical carbon atoms located at

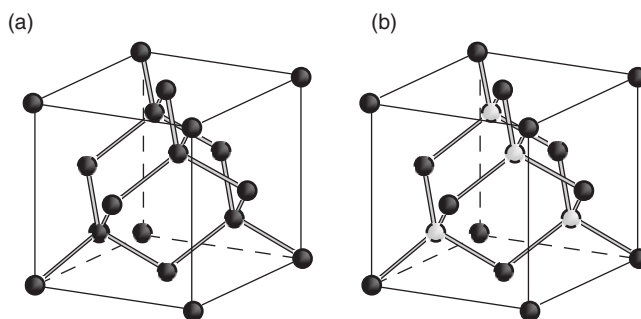


Figure 1.11

Crystal structure (FC cubic) of (a) diamond and (b) zinblende (ZnS).

$$\begin{aligned}\vec{R}_1 &= 0\vec{a}_1 + 0\vec{a}_2 + 0\vec{a}_3 \\ \vec{R}_2 &= \frac{1}{4}\vec{a}_1 + \frac{1}{4}\vec{a}_2 + \frac{1}{4}\vec{a}_3\end{aligned}\quad (1.10)$$

Zincblende (ZnS), shown in Fig. 1.11b, is identical in structure to that of diamond, except that the basis contains two dissimilar atoms:

$$\begin{aligned}\vec{R}_S &= 0\vec{a}_1 + 0\vec{a}_2 + 0\vec{a}_3 \\ \vec{R}_{Zn} &= \frac{1}{4}\vec{a}_1 + \frac{1}{4}\vec{a}_2 + \frac{1}{4}\vec{a}_3\end{aligned}\quad (1.11)$$

1.3.2 Hexagonal lattices

The primitive cell of the hexagonal space lattice, shown in Fig. 1.12a, looks nothing at all like a hexagon. Instead it resembles a tall rectangular box that has been squished from four 90° angles to a pair of 120° and 60° angles, respectively. The hexagonal appearance only emerges when three or more of these boxes are combined.

Hexagonal close packed (HCP)

By far the most prominent occurrence of hexagonal structure in nature appears in the form of the *hexagonal close packed* (HCP) structure in which the

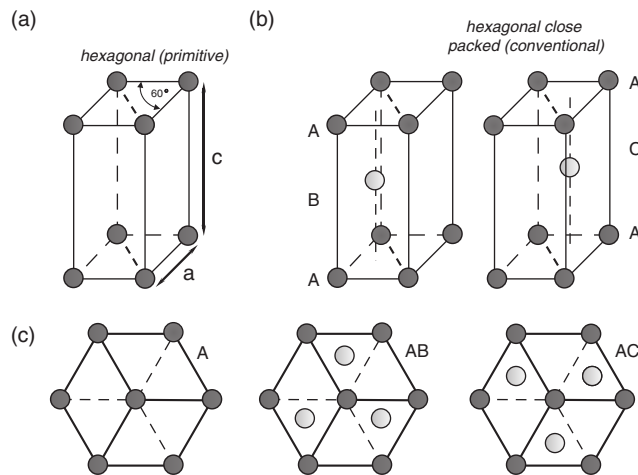


Figure 1.12

(a) Primitive cell of the hexagonal lattice and (b) corresponding conventional cells for the hexagonal close packed structure. The two conventional cells differ only in the location of the central lattice site (B versus C). (c) Three conventional cells are combined to form a hexagonal base (A) with two possibilities for the central layer (AB versus AC).

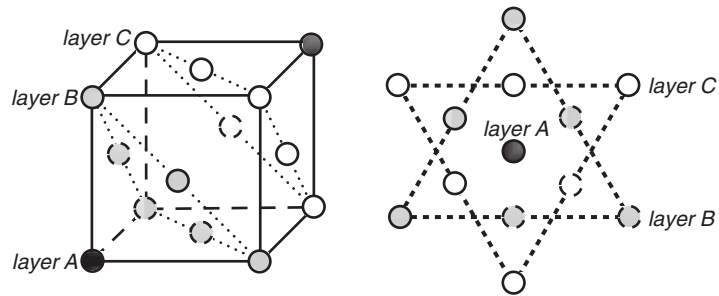


Figure 1.13

The lattice sites of a conventional FCC cubic lattice (left-hand figure) are shown to be equivalent to the lattice sites of the hexagonal layering ABCABC

primitive cell contains a two particle basis. As shown in Fig. 1.12b, the second particle is located on one side or the other of the squished box midway up. The simplest way to view the HCP structure is to consider that it is constructed by alternating layers of the 2D hexagonal lattice. When we combine three primitive cells each with two basis particles, our bottom layer (layer A) appears as a hexagonal net (see Fig. 1.2c). The next layer (layer B) is formed by the second particle of the basis and again forms another hexagonal net which is *offset* from layer A such that the particles in layer B minimize waste space by fitting into some of the shallows of layer A. If the second particle in the basis set happened to be located on the other side of the primitive cell, an alternative layer (layer C) could likewise be positioned atop layer A. In either case, the second layer is then covered by another layer A, directly over the first layer, which corresponds to the top of the three primitive cells.

Layering of the form ABABAB . . . or ACACAC . . . makes up the HCP structure. But layering of the form ABCABC . . . does not! As shown in Fig. 1.13, this third layering pattern just reproduces the FCC structure. The packing fractions of the HCP and FCC are identical and both correspond to the best packing efficiency possible for an ordered arrangement of spheres.

Summary

- The arrangement of atoms in any ideal crystal can be described by a combination of a space lattice (defined by the set of translations, $\vec{T} = h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$) and a basis set (defined in reference to a lattice site by $\vec{R}_i = x_i\vec{a}_1 + y_i\vec{a}_2 + z_i\vec{a}_3$) affixed to each lattice site.
- A primitive cell contains only one lattice site and has the smallest volume needed to fill space by the translations, \vec{T} . Conventional cells contain more than one lattice site.

- Space lattices are categorized according to their special symmetry properties into 14 distinct types known as Bravais lattices.
- The ideal packing fraction is the ratio of cell space occupied by a monatomic basis with atoms of maximal diameter to the volume of the cell itself.
- The coordination number refers to the number of neighboring lattice sites located at a common distance from a central site.

Exercises

- 1.1. Show that the volume of the primitive cell of a BCC crystal lattice is $a^3/2$, where a is the lattice constant of the conventional cell.
- 1.2. Show that the volume of the primitive cell of a FCC crystal lattice is $a^3/4$, where a is the lattice constant of the conventional cell.
- 1.3. Show that the packing fraction of a BCC crystal lattice is $\sqrt{3}\pi/8 = 0.680$.
- 1.4. Show that the packing fraction of a FCC crystal lattice is $\sqrt{2}\pi/6 = 0.740$.
- 1.5. The 2D crystal shown in Fig. 1.14 contains three atoms with a chemical formula ABC_2 . Illustrated in the figure are several possible tiles. (a) Identify which of the tiles are primitive cells. (b) Identify which of the tiles are conventional cells. (c) Identify any tiles that are unable to correctly fill the space. (d) For each primitive cell, provide expressions for the appropriate basis vectors describing the basis set of atoms.

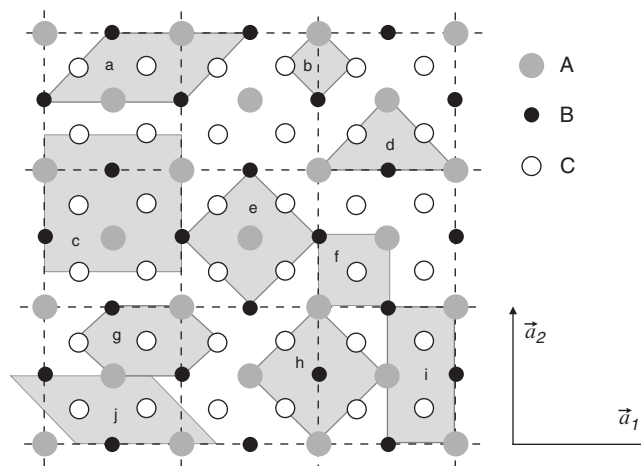


Figure 1.14

- 1.6. Consider again the 2D crystal shown in Fig. 1.14. Describe all the basic symmetry operations (translation, rotation and mirror only) satisfied by this lattice.
- 1.7. For the HCP crystal structure, show that the ideal c/a ratio is 1.633.
- 1.8. Bromine has an orthorhombic lattice structure with $|\vec{a}_1| = 4.65 \text{ \AA}$, $|\vec{a}_2| = 6.73 \text{ \AA}$, $|\vec{a}_3| = 8.70 \text{ \AA}$. (a) The atomic weight of bromine is 79.9 g/mol. If it has a density of 3.12 g/cc, how many bromine atoms reside in a single unit cell? (b) Which type of orthorhombic lattice (i.e. BC, FC, etc.) is suggested by your finding in part (a)? Explain. (c) If the atomic radius of bromine is 1.51 Å, determine the packing fraction.
- 1.9. Shown in Fig. 1.15 is the unit cell of a monatomic crystal. (a) How would you describe this particular crystal structure? (b) What is the maximum packing fraction you should expect for this specific structure?

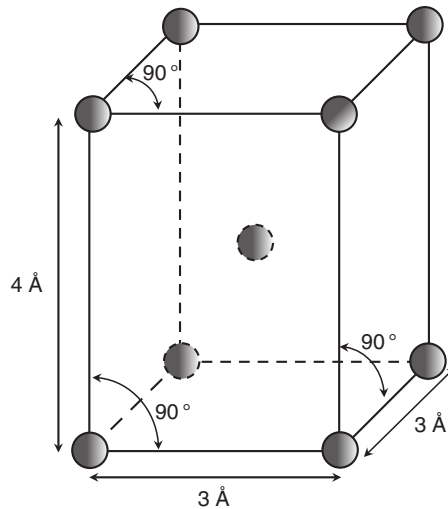


Figure 1.15

Suggested reading

There are many good introductory textbooks that develop crystal structure. These are just a few favorites:

- C. Kittel, *Introduction to Solid State Physics*, 8th Ed. (John Wiley and Sons, 2005).
- J. S. Blakemore, *Solid State Physics*, 2nd Ed. (W. B. Saunders Co., Philadelphia, 1974).
- N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehart and Winston, New York, 1976).
- M. A. Omar, *Elementary Solid State Physics: Principles and Applications* (Addison-Wesley, Reading, MA, 1975).