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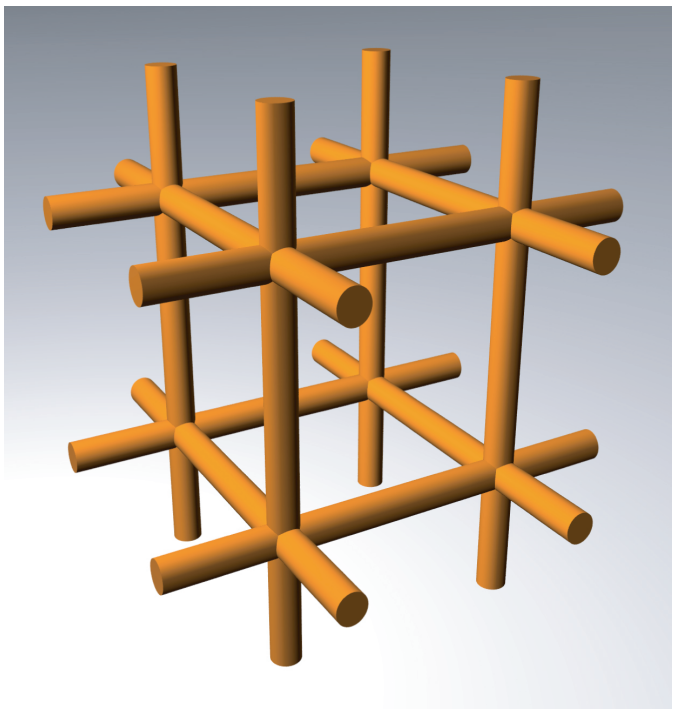
Structural Periodicity



Nature is replete with fascinating examples of intricate structures. The goal of several disciplines in the physical sciences is to control and exploit the function and properties of natural and engineered structures. The first step of such an effort is to have an approach that allows us to understand, characterize, and mathematically describe any general structure. To make a start at such an ambitious effort, we focus on trying to describe one particular subset, viz. periodic structures.

Periodic Materials and Interference Lithography. M. Maldovan and E. Thomas

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1.1 Nonperiodic versus Periodic Structures

Nature attracts the attention of scientists and engineers with multiple examples of outstanding structures that fulfill specific demands. For example, wood has a huge capacity to carry sustained loads and has extraordinary mechanical properties due to a delicate action between fibers of cellulose, hemicellulose, and lignin. Another example of a fibrous natural structure that meets several specific demands is bone, which moves, supports, and protects the body of vertebrates and achieves all these functionalities by being strong and lightweight at the same time. Nature also provides wonderful examples of structures that are built by insects and animals. A supreme example of insect engineering is the honeycomb structure in bee hives, which is made of perfectly uniform repetitive cells that are efficiently organized in space to raise the young bees.

Scientists and engineers have always had curiosity for naturally occurring structures and have been *borrowing* ideas from nature since early days. Needless to say that nature has had plenty of time to develop its structural designs, whereas scientists and engineers can be considered as relative beginners in this field. Nevertheless, scientists and engineers have been successful in replicating some naturally occurring structures, but equally important, they have come up with their own structural designs that meet specific *human* demands.

We do not have to look very far to see the results of the inspiration of engineers for structures. Bridges and tall buildings that can support large loads and stand safely for years are extraordinary examples of engineering achievement and design. At smaller length scales, scientists and engineers have recently designed and fabricated structures that can interact with acoustic and electromagnetic waves in such a way that sound and light can be totally reflected by the structures. Unfortunately, the length scales of these structures do not allow for human visual perception, and so substantial magnification is needed to visualize the architectures (e.g. scanning electron microscopes with magnifications in excess of 100 000×).

Irrespective of the scale at which the structure is built, natural and man-made structures can be classified into two distinct groups: *nonperiodic* and *periodic* structures. In the first case, the structure consists of elements forming a disordered arrangement, thus lacking organization or regularity in space. In the second case, however, the structure is made of a basic object that repeats at precise intervals in space and the resultant structure possesses regularity (Figure 1.1).

Illustrative examples of nonperiodic solid structures are metallic or polymeric foams. These foams are basically created by injecting a low-pressure inert gas into a melted metal or polymer. After solidification, the mixture forms a disordered structure where many gas bubbles are trapped in the solid. The bubbles are nearly randomly distributed within the structure and they may be of various sizes (e.g. different radius in the case of spheres). Some polymeric foams are widely used as packing materials, while other polymeric or metallic foams are used for sound absorption in acoustical insulators or for low thermal conductivity in thermal insulators.

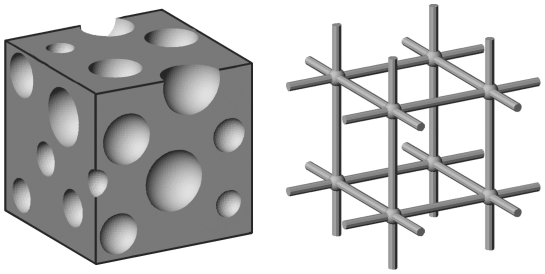


Fig. 1.1 (a) A three-dimensional *nonperiodic* structure made of various size gas bubbles randomly distributed within a solid material. (b) A portion of a three-dimensional infinite *periodic* structure created by a regular repetition of an object in space.

The theoretical prediction of the physical properties of nonperiodic structures is difficult. In fact, theoretical results for such structures are not exact and intense computational methods are required for understanding the complex relationship between structure and physical properties. For example, to properly study the physical properties of a nonperiodic structure, a large portion of the structure must be considered. If this portion is too small, the numerical results will not correspond to the actual properties of the structure. This becomes obvious in the limiting case, since, for example, the consideration of a single bubble cannot be regarded as an accurate description of a structure where many bubbles of different sizes are irregularly distributed in space. In addition to this size effect, it is also difficult to determine the number of different computational *samples* that need to be studied to obtain accurate properties. For example, one computational sample may contain numerous bubbles with large radius, whereas other samples may contain only a few. To obtain precise numerical calculations, it is therefore needed to study many computational samples consisting of randomly located bubbles with different radius and determine the physical properties statistically. This makes the theoretical prediction of the physical properties of nonperiodic structures even more difficult.

On the other hand, we have periodic structures, which are created by a regular repetition of an object in space. The frame figure provided at the beginning of this chapter, comprising a set of uniform beams having a fixed distance among them, is an example of a periodic structure. On large scales, examples of periodic structures include scaffold structures or building frameworks where the constituent objects (e.g. beams and columns) are regularly distributed in space and all have the same size. The theoretical prediction of the properties of periodic structures is less difficult than in the case of nonperiodic structures. Since the structure is formed by a repeating object, all the information needed to describe the entire structure is given by the object itself and by the manner it repeats in space. As a result, only a small portion of the structure (which includes the repeating object) needs to be considered to obtain the properties of the whole periodic structure. The application

of periodic boundary conditions to this small portion of the structure allows for less complicated numerical techniques to obtain precise relationships between structure and physical properties. Moreover, in the case of periodic structures, only a single computational *sample* needs to be studied because the sample precisely describes the periodic structure, as the object that repeats in space is always of the same size.

Nonperiodic and periodic structures are both important from the point of view of practical applications. In this book, we focus on periodic structures for a number of reasons: First, periodic structures have recently shown strikingly new physical properties that permit control of elastic and electromagnetic waves. Second, an experimental technique is currently available that allows engineers to fabricate periodic structures while having certain control over the geometry of the resultant structure. Finally, there are several numerical techniques that can be used to predict the physical properties of periodic structures, which in turn allow us to design, understand, and optimize the structures prior to their experimental fabrication. All these considerations are explained throughout this book. To start studying periodic structures, we first introduce a theoretical scheme to represent and classify periodic structures.

1.2
Two-dimensional Point Lattices

In this book, we are interested in how the geometry of a periodic structure determines the resultant physical properties of the structure. To achieve this, we need a framework that allows us to classify and systematically specify the large number of possible periodic structures. In this section, we introduce an abstract model, called the *point lattice model*, that classifies periodic structures in terms of how they repeat in space.

In the text that follows, we begin with the description of two-dimensional periodic structures because the graphical representation of these structures is simpler than that of the three-dimensional case. The extension to three dimensions is then made by generalizing the concepts developed for the two-dimensional case.

A periodic structure may be defined as an assembly of an *object* that repeats regularly in space. For example, consider the two-dimensional periodic structure represented in Figure 1.2a, which is considered to extend infinitely in the plane. The structure can be divided by two sets of equally spaced parallel lines (Figure 1.2b). This division of the structure produces a set of objects, each of which is identical in size and shape. One of these constituent objects is shown in dark gray in Figure 1.2b. As a result, the two-dimensional periodic structure can be understood as formed by the regular repetition of this object in space. Note that the equally spaced parallel lines also generate a set of two-dimensional cells within which the objects are enclosed.

To understand periodic structures, it is useful, for the moment, to consider each object as an imaginary point. This consideration transforms the periodic structure into an infinite array of equivalent points (Figure 1.2c). The corresponding array

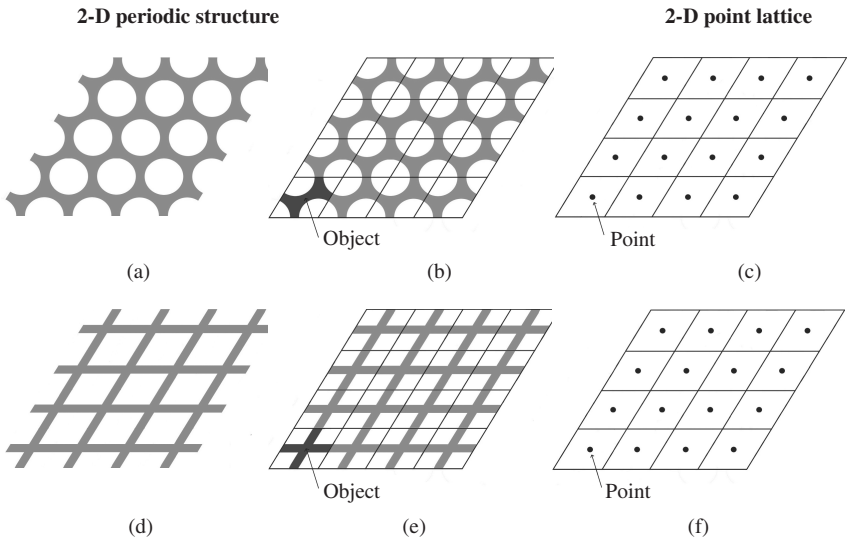


Fig. 1.2 A two-dimensional periodic structure and its point lattice. (a and d) Two distinct two-dimensional periodic structures. (b and e) The structures are divided by equally spaced parallel lines that define the object that repeats in space. (c and f) The object is represented by an imaginary point at its center and the two-dimensional periodic structure transforms into the corresponding point lattice.

of points is called the *point lattice* of the structure, and basically determines the positions of the repeating objects. Hence, the existence of spatial periodicity in the structure implies that the structure has a periodic array of lattice points associated with it. Note that the surroundings viewed from an arbitrary point in the point lattice are identical to the surroundings viewed from any other point. That is, each point in a point lattice has identical surroundings.[1)]

Figure 1.2d shows a different two-dimensional periodic structure. The point lattice associated with this structure, however, is the same as the one corresponding to the structure shown in Figure 1.2a. After dividing the structure by two sets of equally spaced parallel lines (Figure 1.2e) and replacing the set of identical objects by imaginary points (Figure 1.2f), the corresponding point lattice is the same as in Figure 1.2c. That is, the periodic structures shown in Figures 1.2a and d have the same point lattice associated with them and thus have *the same spatial periodicity*. This is due to the fact that the objects corresponding to each structure repeat similarly in space.

Even though each two-dimensional periodic structure has a specific point lattice associated with it, the point lattice can be displayed in various ways. For example,

1) The position (relative to the underlying structure) of the two sets of equally spaced parallel lines that enclose the repeating object in Figure 1.2b is arbitrary. Therefore, the definition of the object that repeats regularly in space to form the periodic structure is also arbitrary. This means that the periodic structure shown in Figure 1.2a can alternatively be described by different choices for the repeating object. The corresponding point lattice, however, is independent on the choice of the particular repeating object.

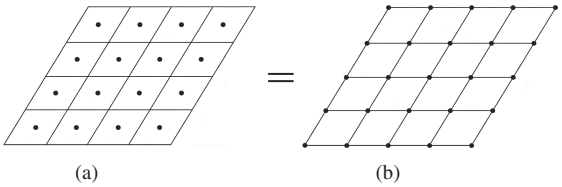


Fig. 1.3 A two-dimensional point lattice with the lattice points located (a) at the center of the cells and (b) at the corner of the cells.

the point lattice shown in Figure 1.3a has the points located at the center of the cells. However, the *same* point lattice can optionally be displayed with the points located at the corners of the cells (Figure 1.3b). In both the cases, the point lattice remains the same. That is, the overall distribution of lattice points in space is not changed. Note that additional lattice points from neighboring cells appear in Figure 1.3b since the periodic point lattice extends infinitely. In this book, we choose to represent point lattices with the points located at the corners of the cells.

Because all cells in Figure 1.3b are equivalent, we can arbitrarily choose any of those cells as a *unit cell* that repeats to form the point lattice. In this particular example, the edges of the unit cells have equal lengths. In the general case, however, the unit cell is an arbitrary parallelogram that can be described by the *primitive vectors* $\mathbf{a}_1$ and $\mathbf{a}_2$ (Figure 1.4), and when repeated by successive translations in space the unit cell forms the corresponding point lattice. The distances $a = |\mathbf{a}_1|$, $b = |\mathbf{a}_2|$, and the angle γ are called the *lattice constants*.

The primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ defining the unit cell also construct the entire point lattice by translations. For example, the point lattice can be viewed as an array of regularly spaced points located at the tip of the vector

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 \tag{1.1}$$

where n_1 and n_2 are arbitrary integer numbers. Equation 1.1 indicates that for each particular set of n_1 and n_2 values there is a corresponding lattice point $\mathbf{R}$ in space. Therefore, the vector $\mathbf{R}$ fills the plane with regularly spaced points and it is said to generate the point lattice.

The number of conceivable two-dimensional periodic structures is infinite. However, when two-dimensional periodic structures are transformed into their

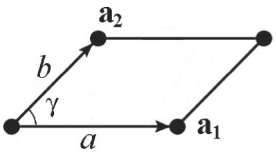


Fig. 1.4 A general two-dimensional unit cell defined by two nonorthogonal vectors, $\mathbf{a}_1$ and $\mathbf{a}_2$.

corresponding point lattices, only five distinct point lattices are found. In other words, the existence of an object that repeats regularly in space, together with the requirement that the repeating objects must have identical surroundings, determines the existence of only five types of point lattices. Therefore, we have achieved one of our goals: *we can classify the infinite set of two-dimensional periodic structures by their spatial periodicity into five categories.*

The five types of two-dimensional point lattices are known as *oblique*, *rectangular*, *square*, *triangular*, and *rhombus* (or centered rectangular). They are illustrated in Figure 1.5 together with the choices for the primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. The distinct geometrical features of the five point lattices are determined by the relative lengths a and b of the primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, and the value of the angle γ. These values

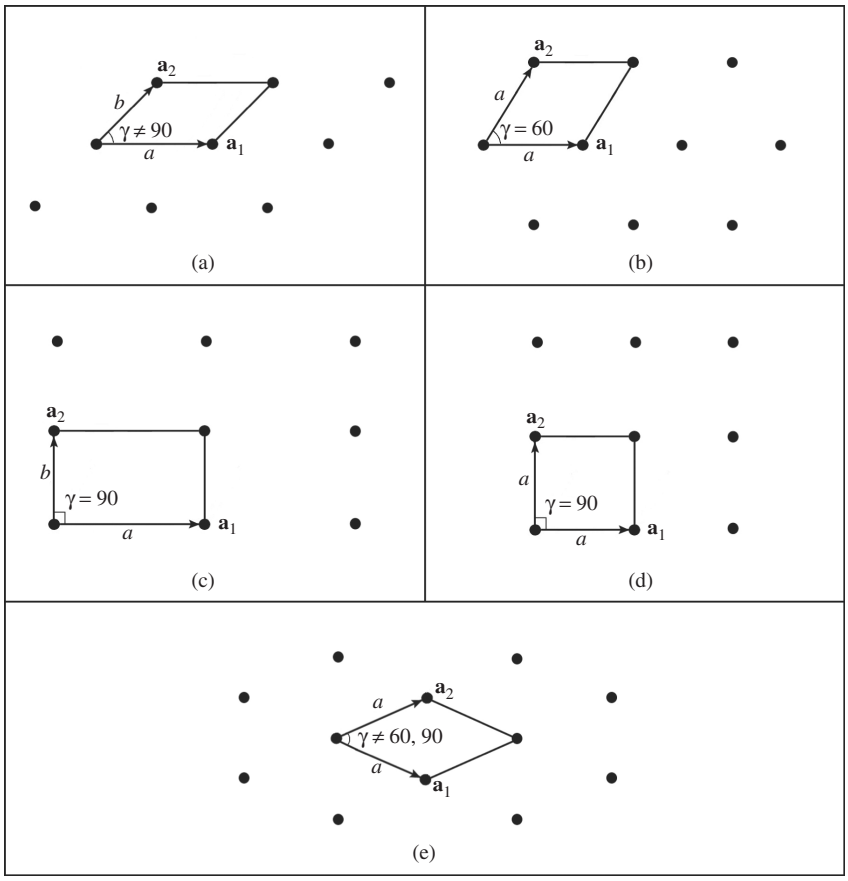


Fig. 1.5 The five two-dimensional point lattices: (a) oblique, (b) triangular, (c) rectangular, (d) square, and (e) rhombus (or centered rectangular).

are given as follows:

- oblique, $a \neq b$, $\gamma \neq 90^\circ$
- rectangular, $a \neq b$, $\gamma = 90^\circ$
- square, $a = b$, $\gamma = 90^\circ$
- triangular, $a = b$, $\gamma = 60^\circ$
- rhombus, $a = b$, $\gamma \neq 60^\circ, 90^\circ$

Note that rectangular, square, triangular, and rhombus lattices can all be considered as special cases of the oblique lattice.

1.3 Three-dimensional Point Lattices

In the previous section, we introduced the principles needed to classify two-dimensional periodic structures in terms of their translational spatial periodicities. In this section, we extend these concepts to the more significant three-dimensional case.

As in the previous section, to classify three-dimensional periodic structures by their translational spatial periodicity, we need to identify within the structure an object that repeats regularly in space. This repeating object is then considered as an imaginary point and the three-dimensional periodic structure transforms into a three-dimensional array of equivalent points. However, to identify and enclose a repeating object in three dimensions, we need to use three sets of equally spaced parallel planes instead of two sets of equally spaced parallel lines as those used in the two-dimensional case.

As an illustrative example, consider the three-dimensional periodic structure shown in Figure 1.6a. The structure is divided by three sets of equally spaced parallel planes (Figure 1.6b). The set of parallel planes identifies the set of objects that repeat regularly in space, each of which is identical in size and shape. The three-dimensional periodic structure is thus constructed by the regular repetition of this object (shown in dark gray in Figure 1.6b). Note that the equally spaced planes also generate a set of three-dimensional cells within which the objects are enclosed. When the repeating object is considered as an imaginary point, the three-dimensional periodic structure transforms into its corresponding point lattice (Figure 1.6c).[2)]

Figures 1.6d–f show the same scheme, but applied to a slightly different three-dimensional periodic structure made of rods connected at right angles. It can be seen that the point lattice associated with this structure is the same as the

2) In analogy with the two-dimensional case, the location (relative to the underlying structure) of the three sets of equally spaced parallel planes that enclose the repeating object in Figure 1.6b is arbitrary. Therefore, the definition of the object that repeats regularly in space is arbitrary and the periodic structure can alternatively be described by different choices for the repeating object. However, the corresponding three-dimensional point lattice is independent on the choice of the repeating object.

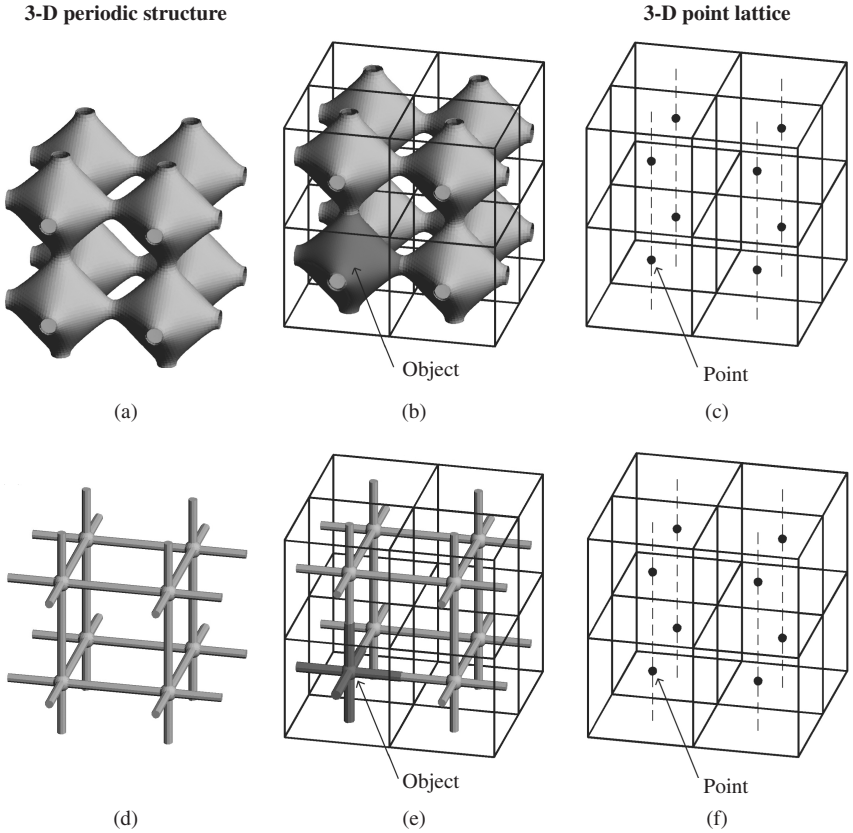


Fig. 1.6 A three-dimensional periodic structure and its point lattice. (a and d) Two different three-dimensional periodic structures. (b and e) The structures are divided by equally spaced parallel planes that define the object that is repeated. (c and f) The object is represented by an imaginary point and the three-dimensional periodic structures transform into their corresponding point lattices.

one corresponding to the previous structure. This is due to the fact that the objects corresponding to each structure repeat similarly in space.

In analogy with the two-dimensional case, three-dimensional point lattices can be displayed in various ways. For example, the point lattice shown in Figure 1.7a is displayed with the points located at the center of the cells, but it can also optionally be displayed with the points located at the corners of the cells (Figure 1.7b). In both cases, the point lattice remains the same. To be consistent with the two-dimensional case, we choose to represent this particular three-dimensional point lattice with the points located at the corners of the cells (Figure 1.7b).

Because the three-dimensional cells shown in Figure 1.7b are equivalent, we can arbitrarily choose any of these cells as a *unit cell* that repeats to form the point lattice. In this particular example, the edges of the unit cells are mutually orthogonal and have equal lengths. In the general case, however, the size and shape of the unit

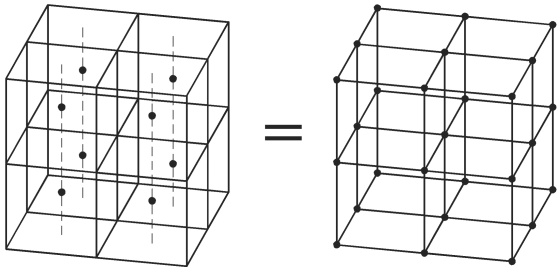


Fig. 1.7 A three-dimensional point lattice with the lattice points located (a) at the center of the cells and (b) at the corner of the cells.

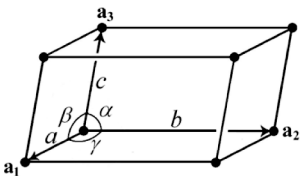


Fig. 1.8 A general three-dimensional unit cell defined by three nonorthogonal vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$.

cell are defined by three nonorthogonal *primitive vectors* $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ (Figure 1.8), where the lengths a, b, and c and the angles α, β, and γ are called the *lattice constants* of the three-dimensional unit cell.

As mentioned in Section 1.2, the primitive vectors can be used to construct the point lattice by translation. For example, a three-dimensional point lattice can be described by an array of regularly spaced points located at the tip of the vector

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{1.2}$$

where n_1, n_2, and n_3 are arbitrary integer numbers. By choosing different values for n_1, n_2, and n_3, the vector $\mathbf{R}$ fills the space with regularly spaced points and generates the corresponding three-dimensional point lattice.

In 1848, the French physicist Bravais demonstrated that there are only 14 possible arrangements of regularly spaced points in space, which satisfy the requirement that each point has identical surroundings. These point lattices were named *Bravais lattices* in his honor. This means that, although the number of conceivable three-dimensional periodic structures is infinite, when three-dimensional periodic structures are transformed into their corresponding point lattices only 14 distinct point lattices are found. Figure 1.9 displays the 14 Bravais lattices using unit cells that are adopted by convention. These *conventional unit cells* easily build up the Bravais lattices by repeating themselves in space, but conventional unit cells do not necessarily have points only at the corners (Figure 1.9). The connection between

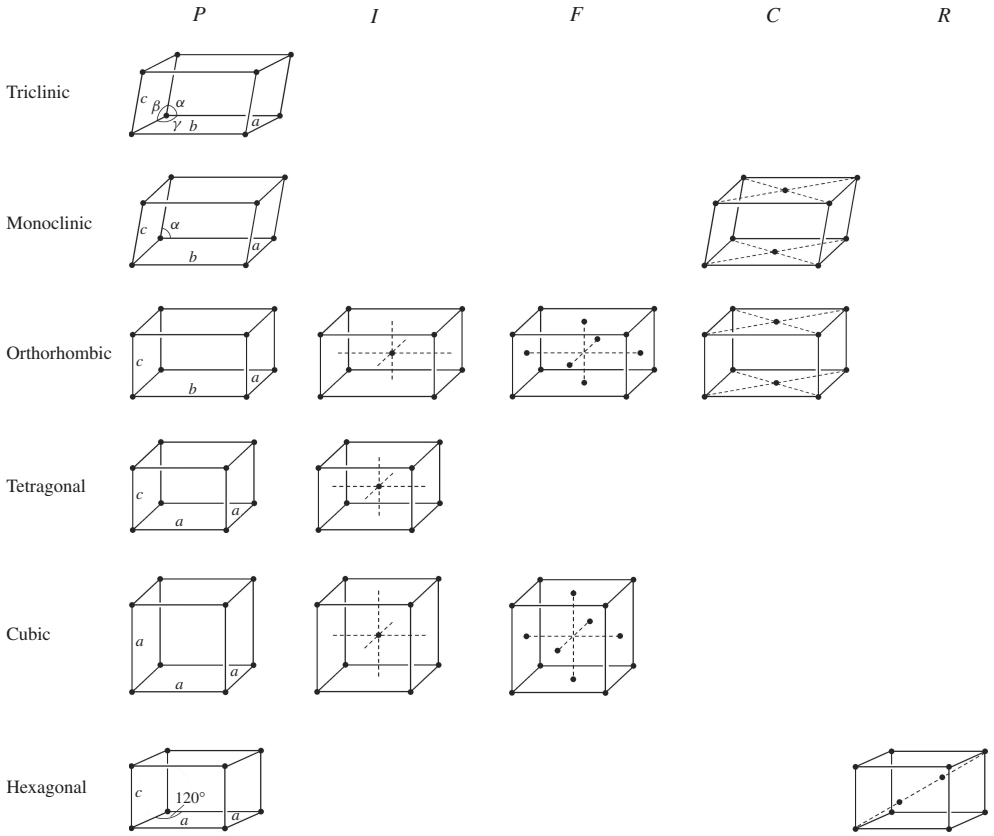


Fig. 1.9 The 14 Bravais lattices. The lattices are grouped in rows according to the shape of the conventional unit cell: triclinic, monoclinic, orthorhombic, tetragonal, cubic, and hexagonal. The six distinct shapes of conventional unit cells define the so-called *six crystal systems*. The lattices are also grouped in columns according to the location of the points within the conventional unit cells.

conventional unit cells and primitive unit cells (which have points only at the corners) is explained in Section 1.3.1.

The 14 Bravais lattices are organized into six *crystal systems*: triclinic, monoclinic, orthorhombic, tetragonal, cubic, and hexagonal. The size and shape of the conventional unit cells used to define the six crystal systems are determined by the relative lengths a, b, and c of the edges of the unit cell and the interaxial angles α, β, and γ (Figure 1.9). These values are given as follows:

- triclinic, $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$
- monoclinic, $a \neq b \neq c$, $\alpha \neq 90^\circ = \beta = \gamma$
- orthorhombic, $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$
- tetragonal, $a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$

- cubic, $a = b = c$, $\alpha = \beta = \gamma = 90^\circ$
- hexagonal, $a = b \neq c$, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$

Note: for simplicity sake, interaxial angles which are equal to 90° are not marked in Figure 1.9.

We can observe different types of conventional unit cells within each crystal system. For example, in the first column the conventional unit cells have points only at the corners of the unit cells. These cells are called *primitive unit cells* and they are designated by the symbol *P*. In the second column, the conventional unit cells have an additional point at the center of the unit cell. In this case, the cells are called *body-centered unit cells* and they are designated by the symbol *I*. In the third column, the cells have additional points at the centers of each face and they are called *face-centered unit cells* and designated by the symbol *F*. In the fourth column, the cells have additional points at the center of two faces. They are called *side-centered unit cells* and are designated by the symbol *C*. Finally, in the last column, the cell contains two additional points located at equal distances along a diagonal of the conventional unit cell. This cell is called a *rhombohedral unit cell* and is designated by the symbol *R*.

We now consider the number of points contained within each type of conventional unit cell. For instance, primitive (*P*) unit cells have points located only at the corners of the unit cells. Since the fractional parts of the points at the corners of the cell always sum to one point within the cell, primitive unit cells have one point per unit cell. Body-centered (*I*) unit cells have an additional point at the center. Hence, this type of unit cell has two points per unit cell. Face-centered (*F*) unit cells have additional points located at the faces, each of which contributes in half to the total number of points. Because there are six faces, the total number of points within the face-centered cells is three (from the faces) + one (from the corners) = four. By following the same reasoning, side-centered (*C*) unit cells have two points per unit cell, whereas rhombohedral (*R*) unit cells have three points per unit cell. Note that the number of points per unit cell is equivalent to the number of objects that are included in the conventional unit cells.

It is important to mention that *any* three-dimensional periodic structure will have one of the 14 Bravais lattices associated with it. To find the Bravais lattice that corresponds to a particular structure, it is only necessary to replace the repeating object in the structure by an imaginary point. Therefore, as we did in the case of two-dimensional periodic structures, *we can classify the infinite set of three-dimensional periodic structures by their spatial periodicity into 14 categories*. On the basis of how the object in the structure repeats in space, the 14 Bravais lattices provide a powerful framework to classify three-dimensional periodic structures.

1.3.1 Primitive and Nonprimitive Unit Cells

We conclude the description of the Bravais lattices by observing the arbitrariness in the choice of the conventional unit cells shown in Figure 1.9. It is important

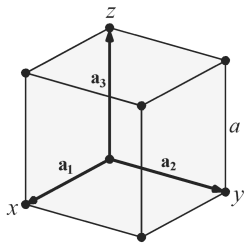
to remark that the arrangement of the regularly spaced points in each of the 14 Bravais lattices is fixed and unique. That is, each Bravais lattice describes a distinct distribution of points in space. However, the unit cell that can be used to graphically represent a Bravais lattice is absolutely arbitrary. We would like to stress the point that the unit cells used to represent the Bravais lattices, shown in Figure 1.9, are chosen by convention to help visualize the symmetric distribution of points (and this explains why they are called *conventional unit cells*).

By definition, the unit cell must construct the Bravais lattice by repeating itself in space. However, nothing is said about the number of points that must be contained within the unit cell. If the unit cell precisely contains a single lattice point, it is called a *primitive unit cell*. For example, unit cells with lattice points only at the corners of the cell are primitive unit cells (first column in Figure 1.9). On the other hand, if the unit cell contains more than one lattice point within the cell, it is called a *nonprimitive unit cell*. For example, the body-centered (*I*), face-centered (*F*), side-centered (*C*), and rhombohedral (*R*) unit cells (Figure 1.9) are nonprimitive unit cells because they contain two, four, two, and three points per unit cell, respectively. Therefore, the conventional unit cells used to represent the 14 Bravais lattices, in Figure 1.9, are primitive in some cases and nonprimitive in others.

It is important to mention, however, that for *any* Bravais lattice we can always find a primitive unit cell to represent the lattice. As an example, we examine in Figure 1.10 the three cubic Bravais lattices. In the first case, the conventional unit cell is a primitive cell, whereas in the case of the face-centered-cubic and body-centered-cubic Bravais lattices, the conventional unit cells are nonprimitive cells. In spite of this, primitive unit cells that describe the corresponding lattices for these two latter cases can be found. Figure 1.10 shows both the conventional nonprimitive and the primitive unit cell for the face-centered-cubic and body-centered-cubic Bravais lattices. The large cubes in solid lines define the conventional nonprimitive unit cells (which contain more than one lattice point), whereas the gray rhombs with six parallelogram faces define the primitive unit cells (which contain a single lattice point). When repeated in space, both the unit cells (nonprimitive and primitive) build up exactly the same lattice. The reason to use the conventional nonprimitive unit cell instead of the primitive unit cell is the fact that the former helps visualize the symmetric distribution of the points in the lattice.

Figure 1.10 also shows the primitive vectors that define the primitive unit cells and generate the corresponding cubic Bravais lattices by the use of Equation 1.2.

To summarize, in the last two sections, we have developed a powerful framework that allows us to classify *any* periodic structure based on its periodicity in space. In the case of two-dimensional structures, in whatever shape or geometry the structure is made, it can be classified into one of the five two-dimensional point lattices (Figure 1.5). On the other hand, in the three-dimensional case, independent of shape or geometry, a three-dimensional structure can always be classified into one of the 14 Bravais lattices (Figure 1.9).

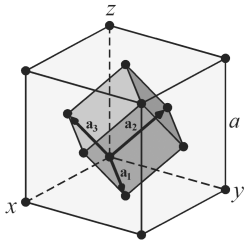


Simple cubic lattice

$$\mathbf{a}_1 = a\,\hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a\,\hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a\,\hat{\mathbf{z}}$$

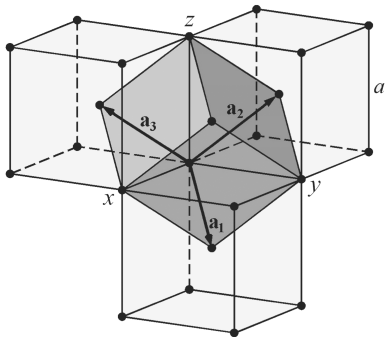


Face-centered-cubic lattice

$$\mathbf{a}_1 = \frac{a}{2}\hat{\mathbf{x}} + \frac{a}{2}\hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{a}{2}\hat{\mathbf{y}} + \frac{a}{2}\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{a}{2}\hat{\mathbf{z}} + \frac{a}{2}\hat{\mathbf{x}}$$



Body-centered-cubic lattice

$$\mathbf{a}_1 = +\frac{a}{2}\hat{\mathbf{x}} + \frac{a}{2}\hat{\mathbf{y}} - \frac{a}{2}\hat{\mathbf{z}}$$

$$\mathbf{a}_2 = -\frac{a}{2}\hat{\mathbf{x}} + \frac{a}{2}\hat{\mathbf{y}} + \frac{a}{2}\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = +\frac{a}{2}\hat{\mathbf{x}} - \frac{a}{2}\hat{\mathbf{y}} + \frac{a}{2}\hat{\mathbf{z}}$$

Fig. 1.10 Simple cubic, face-centered-cubic, and body-centered-cubic Bravais lattices. The face-centered-cubic and body-centered-cubic Bravais lattices can be equivalently represented by a conventional nonprimitive unit cell (large cube) or a primitive unit cell (gray rhomb). The primitive vectors, which define the primitive unit cells, are in the right column.

1.4 Mathematical Description of Periodic Structures

Now that we have a graphic picture of translationally periodic structures we next focus on a mathematical grounding. In the next sections, we describe periodic structures by using analytical formulas. As we show in subsequent chapters, this analytical approach allows us to design periodic structures that can be fabricated by a low-cost experimental technique known as *interference lithography*.

We have shown that the point lattices determine the positions of the object that repeats in space to form two- and three-dimensional periodic structures. In fact, the object is considered to be a point in the abstract lattice model. In this section, we consider the repeating object as a full component having a definite shape. That is, *to classify periodic structures in terms of translational spatial periodicities, the repeating object is considered as an imaginary point, whereas to describe analytically periodic structures the whole object is considered*.

We are interested in periodic structures made of two different constituent materials. These types of structures are called *binary composite structures*. The constituent materials A and B can be *any* type of material (including solids and/or fluids). For example, the composite structure can be made of two different solid materials or of a combination of solid and fluid materials. The aim of this section is to present a method that permits us to quantitatively describe the distribution of materials A and B in a periodic structure by using an analytical function.

Consider a real function $f(x, y)$ defined within a two-dimensional unit cell and assume that the function $f(x, y)$ is positive in some regions and negative in others. By considering that the regions for which $f(x, y)$ is greater than zero are made of material A and that the regions for which $f(x, y)$ is less than zero are made of material B, we have a simple scheme to define the distribution of materials A and B within the unit cell. In fact, the contour line $f(x, y) = 0$ divides the two-dimensional unit cell in regions filled with materials A and B, respectively. Since the two-dimensional unit cell repeats indefinitely in space to form the infinite periodic structure, we are defining the distribution of materials A and B for the whole periodic structure. Analogously, in the case of three-dimensional periodic structures, the scheme can be applied by considering a real function $f(x, y, z)$ and assuming that if $f(x, y, z)$ is greater than zero, the space is filled with material A, whereas if $f(x, y, z)$ is less than zero, the space is filled with material B. In this case, the three-dimensional surface $f(x, y, z) = 0$ divides the space into regions filled with materials A and B.

Therefore, the distribution of materials A and B within the unit cell of a periodic structure (and consequently within the whole structure) is defined as follows:

Two-dimensional structure

$$\text{If} \quad f(x, y) > 0 \Rightarrow \text{Material A} \tag{1.3a}$$

$$\text{If} \quad f(x, y) < 0 \Rightarrow \text{Material B} \tag{1.3b}$$

Three-dimensional structure

$$\text{If} \quad f(x, y, z) > 0 \Rightarrow \text{Material A} \tag{1.4a}$$

$$\text{If} \quad f(x, y, z) < 0 \Rightarrow \text{Material B} \tag{1.4b}$$

Equations 1.3 and 1.4 determine that the analytical description of a periodic structure is now dependent on the definition of the real function $f(x, y, z)$ within the unit cell of structure. (Note: in the rest of this section we focus on the three-dimensional case.)

There exist two inverse situations. On the one hand, we can have some specific periodic structure that is to be described analytically and we want to find the real function $f(x, y, z)$ that represents the structure by the use of Equations 1.4. On the other hand, we can have a real function $f(x, y, z)$ defined within a unit cell and we want to find the geometry of the corresponding periodic structure, which is determined by Equations 1.4. These two inverse situations are as follows:

$$\begin{aligned} &\text{Periodic structure} \longrightarrow \text{corresponding real function } f(x, y, z) \\ &\text{Real function } f(x, y, z) \longrightarrow \text{corresponding periodic structure} \end{aligned}$$

To better understand this important concept, we next consider one example of each case. We first show the case in which we want to find the function $f(x, y, z)$ that describes a particular periodic structure. For example, consider a periodic structure made of solid spheres in air as in Figure 1.11a. This structure is shown in Figure 1.11b together with the planes that define the repeating object (the sphere) and the unit cells. The corresponding simple cubic Bravais lattice is shown in Figure 1.11c.

As previously mentioned, we need to describe the structure only within a single unit cell because the unit cell repeats itself in space to form the periodic structure. Figure 1.12a shows the unit cell of this structure in a Cartesian coordinate system. The center of the sphere is located at $(x_0, y_0, z_0) = (a/2, a/2, a/2)$, where a is the lattice constant of the cubic unit cell. Because the spheres in Figure 1.11a are in contact, the radius of the sphere in Figure 1.12a is $R = a/2$.

We consider that the sphere is made of material B, whereas the background is made of material A. Therefore, the set of points (x, y, z) in the unit cell for which the distance d to the center of the sphere (x_0, y_0, z_0) is less than the radius R form

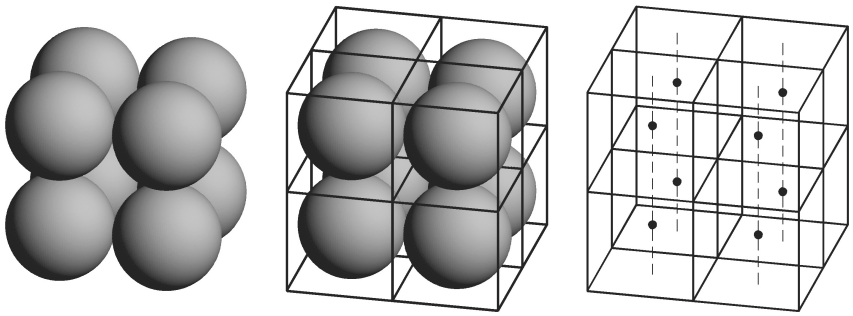


Fig. 1.11 (a) A three-dimensional periodic structure made of solid spheres in air. (b) The structure is divided by equally spaced parallel planes that define the basic object (which in this case is a sphere) and the unit cells. (c) The corresponding simple cubic Bravais lattice. Note that there is one lattice point per unit cell, but our choice here is nonconventional.

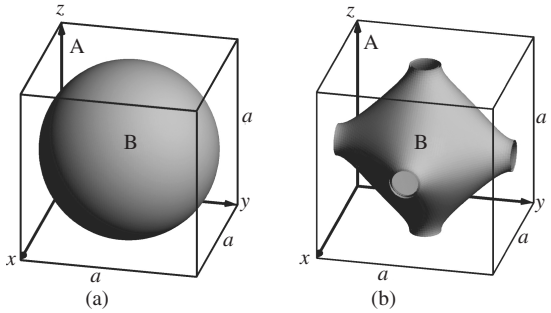


Fig. 1.12 Analytical representation of periodic structures. The distribution of materials A and B within the unit cell of the structure is determined by a function $f(x, y, z)$ together with the inequalities $f(x, y, z) > 0 \Rightarrow$ material A; $f(x, y, z) < 0 \Rightarrow$ material B. (a) $f(x, y, z) = \sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2} - R$, where $(x_0, y_0, z_0) = (a/2, a/2, a/2)$ and $R = a/2$. (b) $f(x, y, z) = \cos(2\pi x/a) + \cos(2\pi y/a) + \cos(2\pi z/a) + 0.85$.

the region filled with material B. On the other hand, the set of points for which the distance d is larger than the radius R form the region filled with material A. This means that the distribution of materials A and B within the unit cell of the structure can be described analytically as follows:

$$\text{If} \quad d = \sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2} > R \Rightarrow \text{Material A} \tag{1.5a}$$

$$\text{If} \quad d = \sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2} < R \Rightarrow \text{Material B} \tag{1.5b}$$

By defining the function

$$f(x, y, z) = \sqrt{(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2} - R \tag{1.6}$$

Equations 1.5 transform into

$$\text{If} \quad f(x, y, z) > 0 \Rightarrow \text{Material A} \tag{1.7a}$$

$$\text{If} \quad f(x, y, z) < 0 \Rightarrow \text{Material B} \tag{1.7b}$$

Therefore, we have succeeded in finding an analytical function $f(x, y, z)$ that describes the periodic structure within the unit cell. We note that this illustrative example is simple due to the fact that the periodic structure is made of spheres. Periodic structures having more complex geometries will certainly require more complicated analytical formulas.

We now consider the inverse case, which is the case frequently found in this book. We have an analytical function $f(x, y, z)$ defined within a unit cell and we want to find the geometry of the periodic structure, which is defined by Equations 1.4. As an illustrative example, consider a function $f(x, y, z)$ made of the sum

of three cosine terms plus a constant defined within a cubic unit cell of lattice constant a

$$f(x,y,z) = \cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{a}\right) + \cos\left(\frac{2\pi z}{a}\right) + 0.85 \tag{1.8}$$

In general, to display the geometry of the periodic structure, we need to use some mathematical software such as Maple, Mathematica, or Matlab. In Figure 1.12b, we show the distribution of materials A and B within the unit cell of the periodic structure defined by Equations 1.4 and the analytical function given in Equation 1.8. In this inverse case, we were thus able to graphically find the geometry of a periodic structure given its analytical formula.

In general, *any* real function $f(x, y, z)$ that changes sign within a unit cell will have associated with it a particular three-dimensional periodic structure defined by Equations 1.4. Owing to the fact that the set of possible analytical functions $f(x, y, z)$ is infinite, the number of periodic structures that can be created by using this scheme is also infinite. In spite of this, in Chapter 2 our main goal is to establish a scheme to *systematically create analytical functions* $f(x, y, z)$ *that represent periodic structures* with the further objective of fabricating these structures by interference lithography. To do this, however, we first need to introduce the Fourier series expansion of a periodic function $f(x, y, z)$, which is a powerful analytical method that is extensively used in Chapter 2 to represent periodic structures.

1.5 Fourier Series

Fourier series is basically a powerful, yet simple mathematical technique that allows us to represent an arbitrary periodic function as a weighted sum of cosine and sine functions. By using this technique, each periodic function has an associated distinctive set of weighted coefficients (or Fourier coefficients) that univocally represent the periodic function. In the next section, we define the Fourier coefficients and show how to calculate them for arbitrary two- and three-dimensional periodic functions.

1.5.1 Fourier Series for Two-dimensional Periodic Functions

Suppose we have a two-dimensional real function $f(x, y)$ defined within a rectangular unit cell of sides a and b. Since the unit cell repeats itself in space to form the periodic structure (Figure 1.13), the function $f(x, y)$ also repeats itself over and over along the x and y directions at intervals of a and b, respectively. This means that

$$f(x + a, y) = f(x, y) \tag{1.9a}$$

$$f(x, y + b) = f(x, y) \tag{1.9b}$$

and the function $f(x, y)$ is said to be *periodic* in two dimensions.

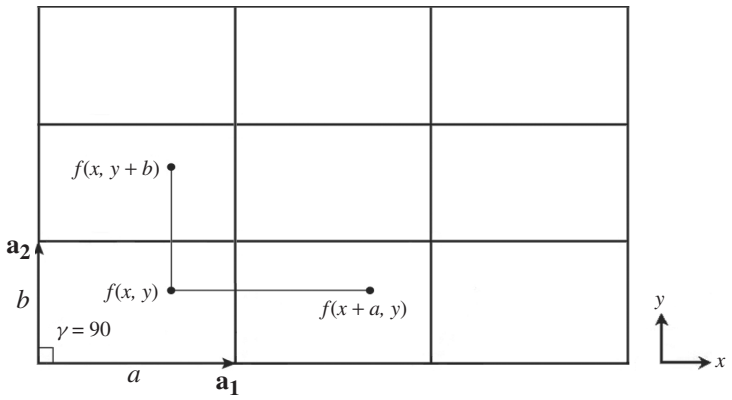


Fig. 1.13 Two-dimensional periodic functions. A function $f(x, y)$ defined within a rectangular unit cell repeats at intervals a and b along the x- and y-axis coordinates, that is, $f(x + a, y) = f(x, y + b) = f(x, y)$. As a result, the function $f(x, y)$ is periodic and it can be represented by its Fourier series expansion.

In general, a two-dimensional *periodic* function $f(x, y)$ can be written as an infinite sum of cosine and sine functions as

$$f(x,y) = a_{00} + \sum_n \sum_m \left\{ a_{nm} \cos\left[2\pi\left(\frac{nx}{a} + \frac{my}{b}\right)\right] + b_{nm} \sin\left[2\pi\left(\frac{nx}{a} + \frac{my}{b}\right)\right]\right\} \tag{1.10}$$

where n and m are integer numbers, a_{00}, a_{nm}, and b_{nm} are real constants, and a and b are the lengths of the sides of the rectangular unit cell. Equation 1.10 is called the *Fourier series expansion* of the periodic function $f(x, y)$, and the constants a_{00}, a_{nm}, and b_{nm} are called the *Fourier coefficients*.

Equation 1.10 establishes that each periodic function $f(x, y)$ has an associated set of Fourier coefficients $\{a_{00}, a_{nm}, b_{nm}\}$. If the formula of the periodic function $f(x, y)$ is known, these coefficients can be obtained by calculating the following integrals.

1.5.1.1 Calculation of a_{00}

By integrating both sides of Equation 1.10 over the area of the rectangular unit cell, we have

$$\int_0^a \int_0^b f(x,y)\,dx\,dy = \int_0^a \int_0^b \left\{ a_{00} + \sum_n \sum_m \left\{ a_{nm} \cos\left[2\pi\left(\frac{nx}{a} + \frac{my}{b}\right)\right] + b_{nm} \sin\left[2\pi\left(\frac{nx}{a} + \frac{my}{b}\right)\right]\right\}\right\} dx\,dy \tag{1.11a}$$

or equivalently

$$\int_0^a \int_0^b f(x,y)\,\mathrm{d}x\,\mathrm{d}y = a_{00}\int_0^a \int_0^b \mathrm{d}x\,\mathrm{d}y + \sum_n \sum_m \left\{ a_{nm} \int_0^a \int_0^b \times \cos\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y + b_{nm}\int_0^a \int_0^b \sin\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y \right\} \tag{1.11b}$$

Because the integrals that contain either cosine or sine functions are equal to zero, independent of the values of n and m, Equation 1.11b determines that

$$a_{00} = \frac{1}{ab}\int_0^a \int_0^b f(x,y)\,\mathrm{d}x\,\mathrm{d}y \tag{1.11c}$$

1.5.1.2 Calculation of a_{nm}

Multiplying Equation 1.10 by $\cos\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]$ and integrating over the area of the rectangular unit cell, we have

$$\int_0^a \int_0^b f(x,y)\cos\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y = \int_0^a \int_0^b \left\{ a_{00} + \sum_n \sum_m \left\{ a_{nm}\cos\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right] + b_{nm}\sin\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\right\}\right\}\cos\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y \tag{1.12a}$$

The integrals on the right-hand side of Equation 1.12a are given by

$$\int_0^a \int_0^b \cos\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y = 0 \qquad \text{for all } n', m' \tag{1.12b}$$

$$\int_0^a \int_0^b \cos\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\cos\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y = \frac{ab}{2}\delta_{n,n'}\,\delta_{m,m'} \tag{1.12c}$$

$$\int_0^a \int_0^b \sin\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\cos\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y = 0 \qquad \text{for all } n, n', m, m' \tag{1.12d}$$

where $\delta_{n,n'}$ is the delta function with properties $\delta_{n,n'} = 1$ if $n = n'$ and $\delta_{n,n'} = 0$ if $n \neq n'$.

By replacing Equations 1.12b–d in Equation 1.12a, the coefficients a_{nm} can be calculated by the integral

$$a_{nm} = \frac{2}{ab}\int_0^a \int_0^b f(x,y)\cos\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y \tag{1.12e}$$

1.5.1.3 Calculation of b_{nm}

Analogously, multiplying Equation 1.10 by $\sin\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]$ and integrating over the area of the rectangular unit cell, we have

$$\begin{aligned}\int_0^a\int_0^b f(x,y)\sin\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y \\ =\int_0^a\int_0^b\left\{a_{00}+\sum_n\sum_m\left\{a_{nm}\cos\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\right.\right. \\ \left.\left.+\ b_{nm}\sin\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\right\}\right\}\sin\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y \qquad (1.13a)\end{aligned}$$

In this case, the integrals on the right-hand side of Equation 1.13a are given by

$$\int_0^a\int_0^b\sin\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y=0 \qquad \text{for all } n',m' \qquad (1.13b)$$

$$\int_0^a\int_0^b\cos\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\sin\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y=0$$
$$\text{for all } n,n',m,m' \qquad (1.13c)$$

$$\int_0^a\int_0^b\sin\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\sin\left[2\pi\left(\frac{n'x}{a}+\frac{m'y}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y=\frac{ab}{2}\delta_{n,n'}\,\delta_{m,m'} \qquad (1.13d)$$

By replacing Equations 1.13b–d in Equation 1.13a, the coefficients b_{nm} can be calculated by the integral

$$b_{nm}=\frac{2}{ab}\int_0^a\int_0^b f(x,y)\sin\left[2\pi\left(\frac{nx}{a}+\frac{my}{b}\right)\right]\mathrm{d}x\,\mathrm{d}y \qquad (1.13e)$$

In summary, Equations 1.11c, 1.12e, and 1.13e determine the set of Fourier coefficients $\{a_{00}, a_{nm}, b_{nm}\}$ associated with the periodic function $f(x, y)$. This set of coefficients univocally define the periodic function $f(x, y)$.

1.5.2 Fourier Series for Three-dimensional Periodic Functions

In complete analogy with the two-dimensional case, consider a three-dimensional real function $f(x, y, z)$ defined within an orthorhombic unit cell of sides a, b, and c. Since the unit cell repeats itself in space to form the periodic structure (Figure 1.14), the function $f(x, y, z)$ also repeats itself over and over along the x, y, and z directions and we have

$$f(x+a,y,z)=f(x,y,z) \qquad (1.14a)$$

$$f(x,y+b,z)=f(x,y,z) \qquad (1.14b)$$

$$f(x,y,z+c)=f(x,y,z) \qquad (1.14c)$$

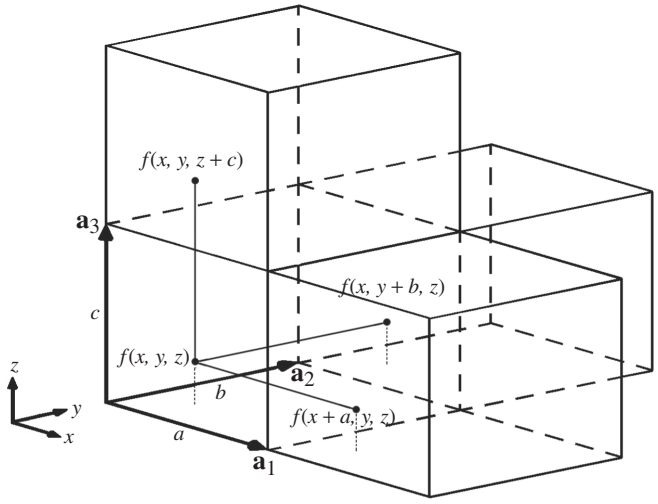


Fig. 1.14 Three-dimensional periodic functions. A function $f(x, y, z)$ defined within an orthorhombic unit cell repeats at intervals a, b, and c along the x-, y-, and z-axis coordinates, that is, $f(x + a, y, z) = f(x, y + b, z) = f(x, y, z + c) = f(x, y, z)$. As a result, the function is periodic and it can be represented by its Fourier series expansion.

Because the function $f(x, y, z)$ is periodic in three dimensions, it can be written as an infinite sum of cosine and sine functions as

$$f(x,y,z) = a_{000} + \sum_n \sum_m \sum_p \left\{ a_{nmp} \cos\left[2\pi\left(\frac{nx}{a} + \frac{my}{b} + \frac{pz}{c}\right)\right] + b_{nmp} \sin\left[2\pi\left(\frac{nx}{a} + \frac{my}{b} + \frac{pz}{c}\right)\right]\right\} \tag{1.15}$$

where n, m, and p are integer numbers, a_{000}, a_{nmp}, and b_{nmp} are the Fourier coefficients, and a, b, and c are the lengths of the edges of the orthorhombic unit cell.

In analogy with the two-dimensional case, the Fourier coefficients a_{000}, a_{nmp}, and b_{nmp} can be calculated by the integrals

$$a_{000} = \frac{1}{abc}\int_0^a \int_0^b \int_0^c f(x,y,z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \tag{1.16a}$$

$$a_{nmp} = \frac{2}{abc}\int_0^a \int_0^b \int_0^c f(x,y,z)\cos\left[2\pi\left(\frac{nx}{a} + \frac{my}{b} + \frac{pz}{c}\right)\right]\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \tag{1.16b}$$

$$b_{nmp} = \frac{2}{abc}\int_0^a \int_0^b \int_0^c f(x,y,z)\sin\left[2\pi\left(\frac{nx}{a} + \frac{my}{b} + \frac{pz}{c}\right)\right]\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \tag{1.16c}$$

For the sake of simplicity, in the last two sections, we considered two- and three-dimensional periodic functions defined within unit cells with mutually orthogonal

edges. This means that, in the two-dimensional case, the periodic functions must be defined within rectangular or square unit cells (Figure 1.5), whereas in the three-dimensional case, the functions must be defined within orthorhombic, tetragonal, or cubic unit cells (Figure 1.9). In the next section, we briefly discuss the Fourier series expansion of a periodic function defined within an arbitrary unit cell, where the angles between the primitive vectors can have arbitrary values.

1.5.3 Arbitrary Unit Cells

Consider a three-dimensional real function $f(\mathbf{r})$ defined within an arbitrary unit cell given by the primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ (Figure 1.8). Here, $\mathbf{r}$ is the position vector $\mathbf{r} = (x, y, z)$. Because the unit cell repeats indefinitely in space, the function $f(\mathbf{r})$ is periodic and satisfies

$$f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R}) \tag{1.17}$$

where $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, and n_1, n_2, and n_3 are arbitrary integer numbers.

A periodic function $f(\mathbf{r})$ defined within an arbitrary unit cell can be written as an infinite sum of cosine and sine functions as

$$f(\mathbf{r}) = a_{000} + \sum_n \sum_m \sum_p \left\{ a_{nmp} \cos\left[\mathbf{G}_{nmp} \cdot \mathbf{r}\right] + b_{nmp} \sin\left[\mathbf{G}_{nmp} \cdot \mathbf{r}\right] \right\} \tag{1.18}$$

where n, m, and p are integer numbers, a_{000}, a_{nmp}, and b_{nmp} are the Fourier coefficients, and $\mathbf{G}_{nmp}$ are called the *reciprocal lattice vectors*. The $\mathbf{G}_{nmp}$ vectors are, in fact, determined by the primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ that define the primitive unit cell. The calculation of the reciprocal lattice vectors $\mathbf{G}_{nmp}$ is introduced in Chapter 6, where general formulas are provided to obtain these vectors from arbitrary unit cells. Equation 1.18 thus represents the Fourier series expansion of a periodic function $f(\mathbf{r})$ defined within an arbitrary unit cell.

To summarize, in this chapter, we introduced the reader to the concept of periodic structures by examining different theoretical aspects. We first examined the notion of spatial periodicity and introduced the point lattice model, which allows us to classify periodic structures depending on how the object that forms the structure repeats itself in space. It turns out that two-dimensional periodic structures can be classified into five two-dimensional point lattices, whereas three-dimensional periodic structures can be classified into 14 three-dimensional Bravais lattices. Then, we examined how periodic structures can be represented by analytical functions. We showed that these analytical functions can in fact be written as a sum of trigonometric terms known as the *Fourier series expansion*. The Fourier series expansion of periodic functions will be the basis to systematically create analytical functions representing periodic structures. We elaborate the procedure in Chapter 2, where we also graphically display the corresponding periodic structures obtained by using this scheme. From this formulation, we arrive at a set of periodic structures that can be fabricated by a currently available experimental technique known as *interference*

lithography and that have applications on a variety of fields that include optics, acoustics, and mechanics.

Further Reading

1 Buerger, M. (**1978**) *Elementary Crystallography: An Introduction to the Fundamental Geometric Features of Crystals*, MIT Press, Massachusetts.

2 Kittel, C. (**1996**) *Introduction to Solid State Physics*, John Wiley & Sons, Ltd, New York.

3 Ashcroft, N.W. and Mermin, N.D. (**1976**) *Solid State Physics*, Saunders College Publishing, New York.

4 Cullity, B.D. (**1978**) *Elements of X-Ray Diffraction*, Addison-Wesley, Massachusetts, Chapter 2.

5 Allen, S.M. and Thomas, E.L. (**1999**) *The Structure of Materials*, John Wiley & Sons, Ltd, New York.

Problems

1.1 Rectangular lattice

(a) Determine the two-dimensional primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ for a rectangular lattice of sides $a = 1.5$ cm and $b = 1$ cm.

(b) By using Equation 1.1, determine the (x, y) positions of the eight nearest points to the origin (0, 0).

(c) Draw the lattice.

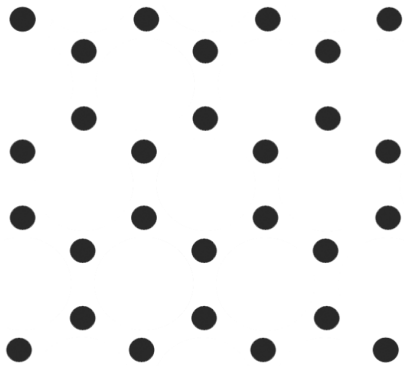
1.2 Triangular lattice

(a) Determine the two-dimensional primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ for a triangular lattice of side $a = 1$ cm.

(b) By using Equation 1.1, determine the (x, y) positions of the six nearest points to the origin (0, 0).

(c) Draw the lattice.

1.3 Why is the following two-dimensional periodic arrangement of points *not* a point lattice?



1.4 Honeycomb structure

(a) On the diagram below, draw two sets of parallel lines to identify and enclose a repeating object that forms the periodic structure.

(b) Replace the repeating object by a point and form the corresponding point lattice. What is the lattice associated with the honeycomb structure?

1.5 Nearest-neighbor points are the points in the Bravais lattice that are closest to a particular point.

(a) Show that the number of nearest-neighbors in the simple cubic, body-centered-cubic, and face-centered-cubic Bravais lattices is 6, 8, and 12, respectively.

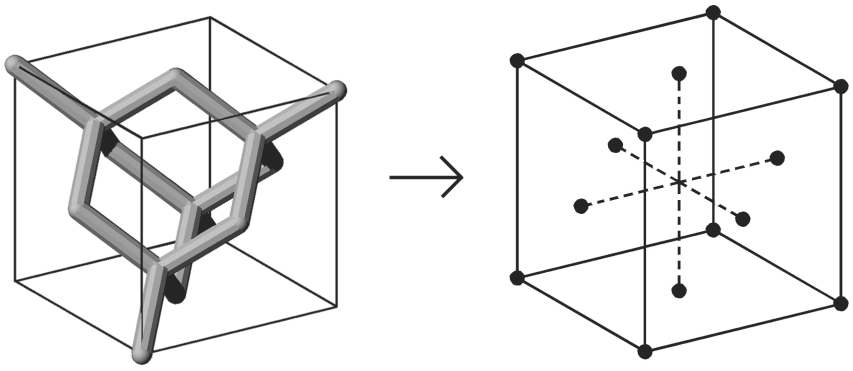
(b) Demonstrate that the distance between nearest-neighbors for the simple cubic, body-centered-cubic, and face-centered-cubic Bravais lattices is a, $\sqrt{3}a/2$, and $\sqrt{2}a/2$, respectively, where a is the lattice constant of the cubic unit cell.

1.6 A diamond structure

(a) In the structure shown below, identify an object that repeats regularly in space to form the three-dimensional diamond structure.

(b) Replace the object by an imaginary point and show that the Bravais lattice associated with the diamond structure is the face-centered-cubic lattice.

Note: the cubic unit cell of the structure repeats infinitely in space.



1.7 Find the function $f(x, y, z)$ that describes the three-dimensional periodic structure shown in Figure 1.6e.

1.8 Sketch the two-dimensional periodic structure described by the function $f(x, y) = \cos(2\pi x) + \cos(2\pi y)$.

1.9 Demonstrate the values of the Integrals 1.12b–d and 1.13b–d. Hint: use the following trigonometric identities

$$\cos\alpha\cos\beta = \tfrac{1}{2}[\cos(\alpha+\beta) + \cos(\alpha-\beta)]$$
$$\sin\alpha\sin\beta = \tfrac{1}{2}[\cos(\alpha-\beta) - \cos(\alpha+\beta)]$$
$$\sin\alpha\cos\beta = \tfrac{1}{2}[\sin(\alpha+\beta) + \sin(\alpha-\beta)]$$

1.10 Calculate the Fourier coefficients $\{a_{00}, a_{nm}, b_{nm}\}$ for a periodic function $f(x, y)$ defined on a square lattice of side a, where

$$f(x,y) = 1 \quad 0.25a < x < 0.75a \quad \text{and} \quad 0.25a < y < 0.75a$$
$$f(x,y) = 0 \qquad\qquad\qquad\qquad \text{otherwise}$$