The Crystal Structure of Solids

This text deals with the electrical properties and characteristics of semiconductor materials and devices. The electrical properties of solids are therefore of primary interest. The semiconductor is in general a single-crystal material. The electrical properties of a single-crystal material are determined not only by the chemical composition but also by the arrangement of atoms in the solid; this being true, a brief study of the crystal structure of solids is warranted. The formation, or growth, of the single-crystal material is an important part of semiconductor technology. A short discussion of several growth techniques is included in this chapter to provide the reader with some of the terminology that describes semiconductor device structures. ∎

1.0 | PREVIEW

In this chapter, we will:

- Describe three classifications of solids—amorphous, polycrystalline, and single crystal.
- Discuss the concept of a unit cell.
- Describe three simple crystal structures and determine the volume and surface density of atoms in each structure.
- Describe the diamond crystal structure.
- Briefly discuss several methods of forming single-crystal semiconductor materials.

1.1 | SEMICONDUCTOR MATERIALS

Semiconductors are a group of materials having conductivities between those of metals and insulators. Two general classifications of semiconductors are the elemental semiconductor materials, found in group IV of the periodic table, and the compound semiconductor materials, most of which are formed from special combinations of group III and group V elements. Table 1.1 shows a portion of the periodic table in

Table 1.1 | A portion of the periodic table

III	IV	V
5 **B** Boron	6 **C** Carbon	
13 **Al** Aluminum	14 **Si** Silicon	15 **P** Phosphorus
31 **Ga** Gallium	32 **Ge** Germanium	33 **As** Arsenic
49 **In** Indium		51 **Sb** Antimony

Table 1.2 | A list of some semiconductor materials

Elemental semiconductors	
Si	Silicon
Ge	Germanium
Compound semiconductors	
AlP	Aluminum phosphide
AlAs	Aluminum arsenide
GaP	Gallium phosphide
GaAs	Gallium arsenide
InP	Indium phosphide

which the more common semiconductors are found and Table 1.2 lists a few of the semiconductor materials. (Semiconductors can also be formed from combinations of group II and group VI elements, but in general these will not be considered in this text.)

The elemental materials, those that are composed of single species of atoms, are silicon and germanium. Silicon is by far the most common semiconductor used in integrated circuits and will be emphasized to a great extent.

The two-element, or *binary,* compounds such as gallium arsenide or gallium phosphide are formed by combining one group III and one group V element. Gallium arsenide is one of the more common of the compound semiconductors. Its good optical properties make it useful in optical devices. GaAs is also used in specialized applications in which, for example, high speed is required.

We can also form a three-element, or *ternary,* compound semiconductor. An example is $Al_xGa_{1-x}As$, in which the subscript x indicates the fraction of the lower atomic number element component. More complex semiconductors can also be formed that provide flexibility when choosing material properties.

1.2 | TYPES OF SOLIDS

Amorphous, polycrystalline, and single crystals are the three general types of solids. Each type is characterized by the size of an ordered region within the material. An ordered region is a spatial volume in which atoms or molecules have a regular geometric arrangement or periodicity. Amorphous materials have order only within a few atomic or molecular dimensions, while polycrystalline materials have a high degree of order over many atomic or molecular dimensions. These ordered regions, or single-crystal regions, vary in size and orientation with respect to one another. The single-crystal regions are called grains and are separated from one another by grain boundaries. Single-crystal materials, ideally, have a high degree of order, or regular geometric periodicity, throughout the entire volume of the material. The advantage of a single-crystal material is that, in general, its electrical properties are superior
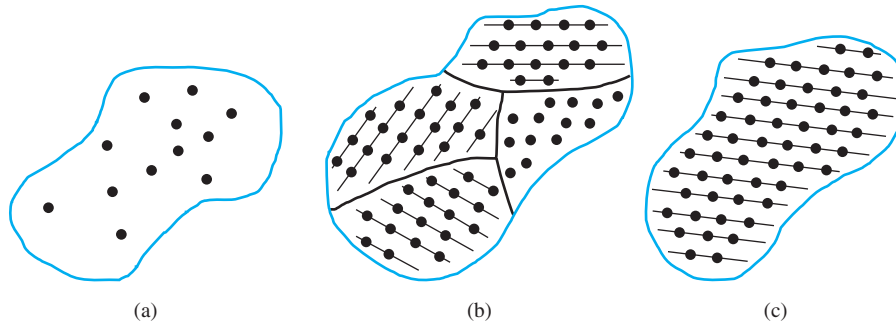
Figure 1.1 | Schematics of three general types of crystals: (a) amorphous, (b) polycrystalline, (c) single.

to those of a nonsingle-crystal material, since grain boundaries tend to degrade the electrical characteristics. Two-dimensional representations of amorphous, polycrystalline, and single-crystal materials are shown in Figure 1.1.

1.3 | SPACE LATTICES

Our primary emphasis in this text will be on the single-crystal material with its regular geometric periodicity in the atomic arrangement. A representative unit, or a group of atoms, is repeated at regular intervals in each of the three dimensions to form the single crystal. The periodic arrangement of atoms in the crystal is called the *lattice*.

1.3.1 Primitive and Unit Cell

We can represent a particular atomic array by a dot that is called a *lattice point*. Figure 1.2 shows an infinite two-dimensional array of lattice points. The simplest means of repeating an atomic array is by translation. Each lattice point in Figure 1.2 can be translated a distance a_1 in one direction and a distance b_1 in a second noncolinear direction to generate the two-dimensional lattice. A third noncolinear translation will produce the three-dimensional lattice. The translation directions need not be perpendicular.

Since the three-dimensional lattice is a periodic repetition of a group of atoms, we do not need to consider the entire lattice, but only a fundamental unit that is being repeated. A *unit cell* is a small volume of the crystal that can be used to reproduce the entire crystal. A unit cell is not a unique entity. Figure 1.3 shows several possible unit cells in a two-dimensional lattice.

The unit cell A can be translated in directions a_2 and b_2, the unit cell B can be translated in directions a_3 and b_3, and the entire two-dimensional lattice can be constructed by the translations of either of these unit cells. The unit cells C and D in Figure 1.3 can also be used to construct the entire lattice by using the appropriate translations. This discussion of two-dimensional unit cells can easily be extended to three dimensions to describe a real single-crystal material.
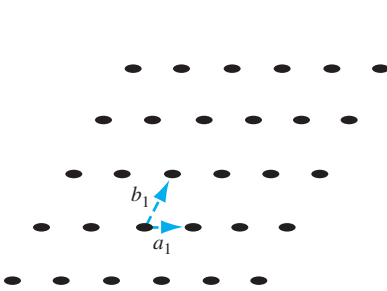
Figure 1.2 | Two-dimensional representation of a single-crystal lattice.
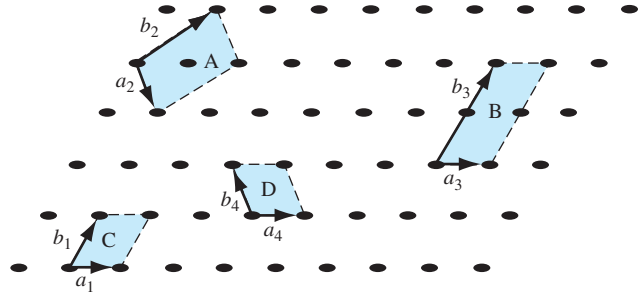
Figure 1.3 | Two-dimensional representation of a single-crystal lattice showing various possible unit cells.

A *primitive cell* is the smallest unit cell that can be repeated to form the lattice. In many cases, it is more convenient to use a unit cell that is not a primitive cell. Unit cells may be chosen that have orthogonal sides, for example, whereas the sides of a primitive cell may be nonorthogonal.

A generalized three-dimensional unit cell is shown in Figure 1.4. The relationship between this cell and the lattice is characterized by three vectors $\bar{a}$, $\bar{b}$, and $\bar{c}$, which need not be perpendicular and which may or may not be equal in length. Every equivalent lattice point in the three-dimensional crystal can be found using the vector

$$\bar{r} = p\bar{a} + q\bar{b} + s\bar{c} \tag{1.1}$$

where p, q, and s are integers. Since the location of the origin is arbitrary, we will let p, q, and s be positive integers for simplicity. The magnitudes of the vectors $\bar{a}$, $\bar{b}$, and $\bar{c}$ are the lattice constants of the unit cell.

1.3.2 Basic Crystal Structures

Before we discuss the semiconductor crystal, let us consider three crystal structures and determine some of the basic characteristics of these crystals. Figure 1.5 shows the simple cubic, body-centered cubic, and face-centered cubic structures. For these simple structures, we may choose unit cells such that the general vectors $\bar{a}$, $\bar{b}$, and $\bar{c}$
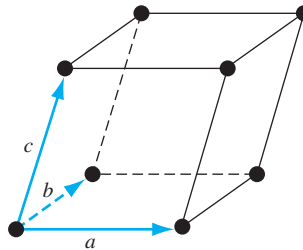
Figure 1.4 | A generalized primitive unit cell.
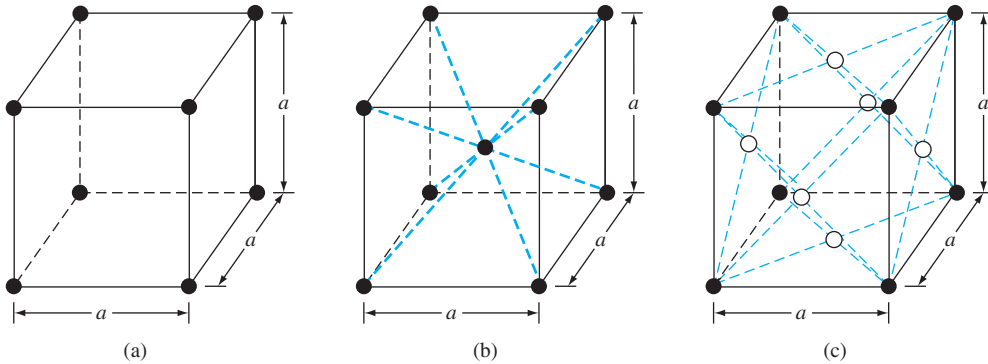
Figure 1.5 | Three lattice types: (a) simple cubic, (b) body-centered cubic, (c) face-centered cubic.

are perpendicular to each other and the lengths are equal. The lattice constant of each unit cell in Figure 1.5 is designated as "*a*." The *simple cubic* (sc) structure has an atom located at each corner; the *body-centered cubic* (bcc) structure has an additional atom at the center of the cube; and the *face-centered cubic* (fcc) structure has additional atoms on each face plane.

   By knowing the crystal structure of a material and its lattice dimensions, we can determine several characteristics of the crystal. For example, we can determine the volume density of atoms.

EXAMPLE 1.1

Objective: Find the volume density of atoms in a crystal.

   Consider a single-crystal material that is a body-centered cubic, as shown in Figure 1.5b, with a lattice constant $a = 5$ Å $= 5 \times 10^{-8}$ cm. A corner atom is shared by eight unit cells that meet at each corner so that each corner atom effectively contributes one-eighth of its volume to each unit cell. The eight corner atoms then contribute an equivalent of one atom to the unit cell. If we add the body-centered atom to the corner atoms, each unit cell contains an equivalent of two atoms.

■ **Solution**
The number of atoms per unit cell is $\frac{1}{8} \times 8 + 1 = 2$

The volume density of atoms is then found as

$$\text{Volume Density} = \frac{\#\ atoms\ per\ unit\ cell}{volume\ of\ unit\ cell}$$

So

$$\text{Volume Density} = \frac{2}{a^3} = \frac{2}{(5 \times 10^{-8})^3} = 1.6 \times 10^{22}\ \text{atoms/cm}^3$$

■ **EXERCISE PROBLEM**

Ex 1.1   The lattice constant of a face-centered cubic lattice is 4.25 Å. Determine the (a) effective number of atoms per unit cell and (b) volume density of atoms.
[Ans. (a) 4; (b) 5.21×10^{22} cm^{-3}]

1.3.3   Crystal Planes and Miller Indices

Since real crystals are not infinitely large, they eventually terminate at a surface. Semiconductor devices are fabricated at or near a surface, so the surface properties may influence the device characteristics. We would like to be able to describe these surfaces in terms of the lattice. Surfaces, or planes through the crystal, can be described by first considering the intercepts of the plane along the $\bar{a}$, $\bar{b}$, and $\bar{c}$ axes used to describe the lattice.

EXAMPLE 1.2

Objective: Describe the plane shown in Figure 1.6. (The lattice points in Figure 1.6 are shown along the $\bar{a}$, $\bar{b}$, and $\bar{c}$ axes only.)
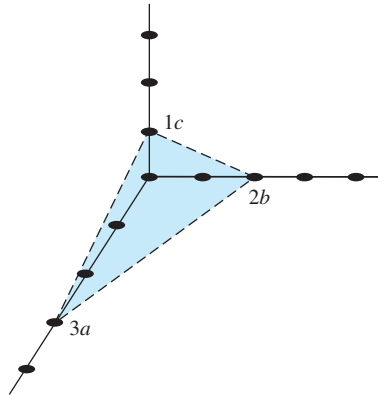
Figure 1.6 | A representative crystal-lattice plane.

■ **Solution**

From Equation (1.1), the intercepts of the plane correspond to $p = 3$, $q = 2$, and $s = 1$. Now write the reciprocals of the intercepts, which gives

$$\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{1} \right)$$

Multiply by the lowest common denominator, which in this case is 6, to obtain (2, 3, 6). The plane in Figure 1.6 is then referred to as the (236) plane. The integers are referred to as the Miller indices. We will refer to a general plane as the (*hkl*) plane.

■ **Comment**

We can show that the same three Miller indices are obtained for any plane that is parallel to the one shown in Figure 1.6. Any parallel plane is entirely equivalent to any other.

■ **EXERCISE PROBLEM**

Ex 1.2   Describe the lattice plane shown in Figure 1.7. [Ans. (211) plane.]
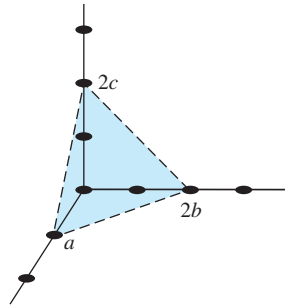
Three planes that are commonly considered in a cubic crystal are shown in Figure 1.8. The plane in Figure 1.8a is parallel to the $\bar{b}$ and $\bar{c}$ axes so the intercepts are given as $p = 1$, $q = \infty$, and $s = \infty$. Taking the reciprocal, we obtain the Miller indices as (1, 0, 0), so the plane shown in Figure 1.8a is referred to as the (100) plane. Again, any plane parallel to the one shown in Figure 1.8a and separated by an integral number of lattice constants is equivalent and is referred to as the (100) plane. One advantage to taking the reciprocal of the intercepts to obtain the Miller indices is that the use of infinity is avoided when describing a plane that is parallel to an axis. If we were to describe a plane passing through the origin of our system, we would obtain infinity as one or more of the Miller indices after taking the reciprocal of the intercepts. However, the location of the origin of our system is entirely arbitrary and so, by translating the origin to another equivalent lattice point, we can avoid the use of infinity in the set of Miller indices.

For the simple cubic structure, the body-centered cubic, and the face-centered cubic, there is a high degree of symmetry. The axes can be rotated by 90° in each

(a)   (b)   (c)
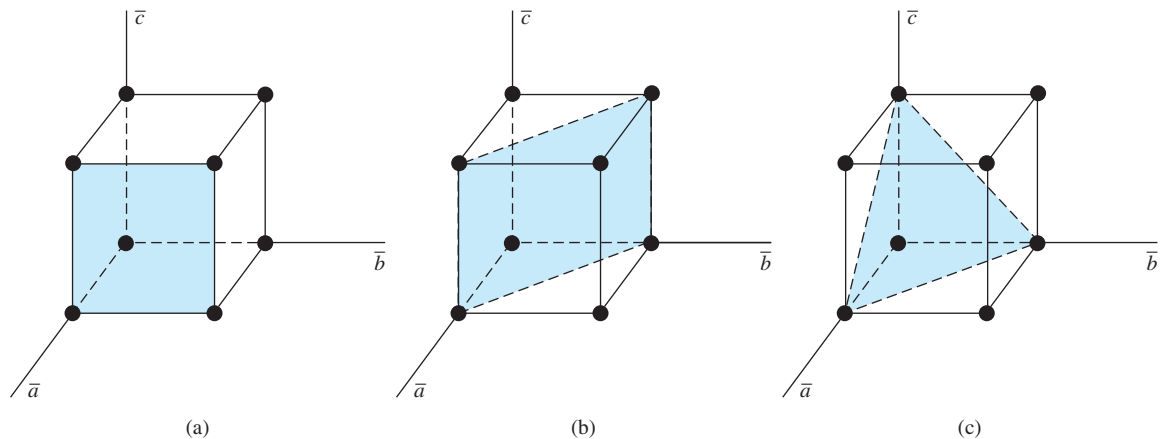
Figure 1.8 | Three lattice planes: (a) (100) plane, (b) (110) plane, (c) (111) plane.

of the three dimensions and each lattice point can again be described by Equation (1.1) as

$$\bar{r} = p\bar{a} + q\bar{b} + s\bar{c} \qquad (1.1)$$

Each face plane of the cubic structure shown in Figure 1.8a is entirely equivalent. These planes are grouped together and are referred to as the {100} set of planes.

We may also consider the planes shown in Figures 1.8b and 1.8c. The intercepts of the plane shown in Figure 1.8b are $p = 1$, $q = 1$, and $s = \infty$. The Miller indices are found by taking the reciprocal of these intercepts and, as a result, this plane is referred to as the (110) plane. In a similar way, the plane shown in Figure 1.8c is referred to as the (111) plane.

One characteristic of a crystal that can be determined is the distance between nearest equivalent parallel planes. Another characteristic is the surface concentration of atoms, number per square centimeter (#/cm²), that are cut by a particular plane. Again, a single-crystal semiconductor is not infinitely large and must terminate at some surface. The surface density of atoms may be important, for example, in determining how another material, such as an insulator, will "fit" on the surface of a semiconductor material.

EXAMPLE 1.3

Objective: Calculate the surface density of atoms on a particular plane in a crystal.

Consider the body-centered cubic structure and the (110) plane shown in Figure 1.9a. Assume the atoms can be represented as hard spheres with the closest atoms touching each other. Assume the lattice constant is $a_1 = 5$ Å. Figure 1.9b shows how the atoms are cut by the (110) plane.

The atom at each corner is shared by four similar equivalent lattice planes, so each corner atom effectively contributes one-fourth of its area to this lattice plane as indicated in the figure. The four corner atoms then effectively contribute one atom to this lattice plane. The atom in the center is completely enclosed in the lattice plane. There is no other equivalent plane that

(a)   (b)
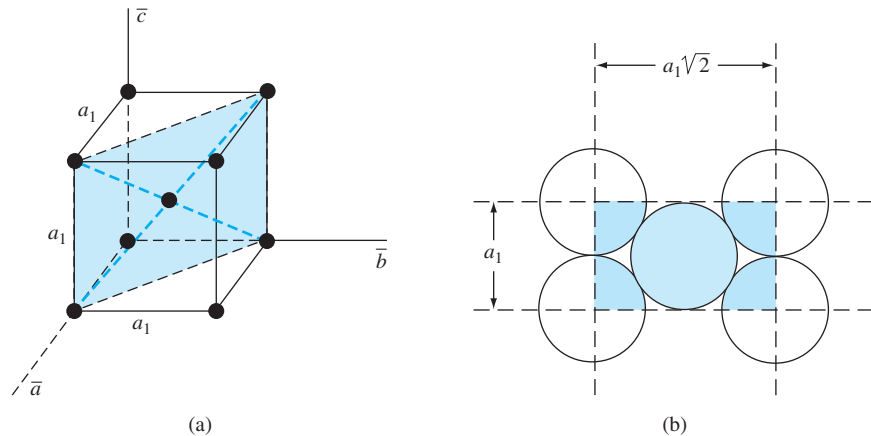
Figure 1.9 | (a) The (110) plane in a body-centered cubic and (b) the atoms cut by the (110) plane in a body-centered cubic.

cuts the center atom and the corner atoms, so the entire center atom is included in the number of atoms in the crystal plane. The lattice plane in Figure 1.9b, then, contains two atoms.

■ **Solution**

The number of atoms per lattice plane is $\frac{1}{4} \times 4 + 1 = 2$

The surface density of atoms is then found as

$$\text{Surface Density} = \frac{\text{\# of atoms per lattice plane}}{\text{area of lattice plane}}$$

So

$$\text{Surface Density} = \frac{2}{(a_1)(a_1\sqrt{2})} = \frac{2}{(5 \times 10^{-8})^2 \sqrt{2}}$$

$$= 5.66 \times 10^{14} \text{ atoms/cm}^2$$

■ **Comment**

The surface density of atoms is a function of the particular crystal plane in the lattice and generally varies from one crystal plane to another.

■ **EXERCISE PROBLEM**

Ex 1.3 The lattice constant of a face-centered-cubic structure is 4.25 Å. Calculate the surface density of atoms for a (a) (100) plane and (b) (110) plane.

[Ans. (a) 1.11×10^{15} cm^{-2}; (b) 7.83×10^{14} cm^{-2}]

1.3.4 Directions in Crystals

In addition to describing crystal planes in a lattice, we may want to describe a particular direction in the crystal. The direction can be expressed as a set of three integers that are the components of a vector in that direction. For example, the body diagonal in a simple cubic lattice is composed of vector components 1, 1, 1. The body diagonal is then described as the [111] direction. The brackets are used to designate direction as distinct from the parentheses used for the crystal planes. The three basic directions and the associated crystal planes for the simple cubic structure are shown in Figure 1.10. Note that in the simple cubic lattices, the [hkl] direction is perpendicular to the (hkl) plane. This perpendicularity may not be true in noncubic lattices.

TEST YOUR UNDERSTANDING

TYU 1.1 The volume density of atoms for a simple cubic lattice is 4×10^{22} cm^{-3}. Assume that the atoms are hard spheres with each atom touching its nearest neighbor. Determine the lattice constant and the radius of the atom. (Ans. $a = 2.92$ Å, $r = 1.46$ Å)

TYU 1.2 Consider a simple cubic structure with a lattice constant of $a = 4.65$ Å. Determine the surface density of atoms in the (a) (100) plane, (b) (110) plane, and (c) (111) plane. [Ans. (a) 4.62×10^{14} cm^{-2}; (b) 3.27×10^{14} cm^{-2}; (c) 2.67×10^{14} cm^{-2}]

TYU 1.3 (a) Determine the distance between nearest (100) planes in a simple cubic lattice with a lattice constant of $a = 4.83$ Å. (b) Repeat part (a) for the (110) plane. [Ans. (a) 4.83 Å; (b) 3.42 Å]
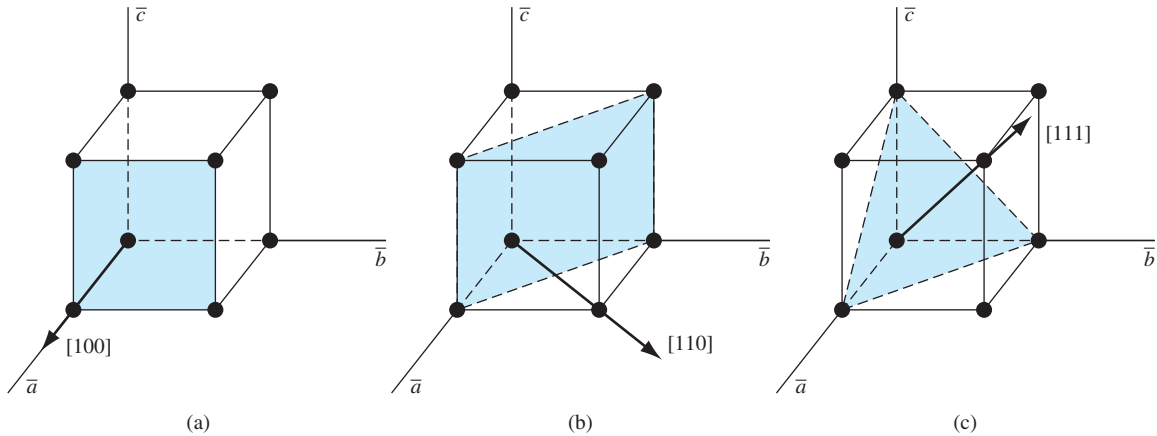
Figure 1.10 | Three lattice directions and planes: (a) (100) plane and [100] direction, (b) (110) plane and [110] direction, (c) (111) plane and [111] direction.
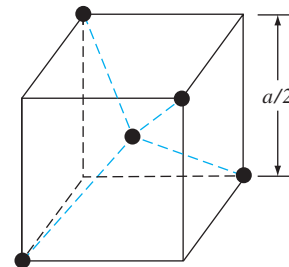
1.4 | THE DIAMOND STRUCTURE

As already stated, silicon is the most common semiconductor material. Silicon is referred to as a group IV element and has a diamond crystal structure. Germanium is also a group IV element and has the same diamond structure. A unit cell of the diamond structure, shown in Figure 1.11, is more complicated than the simple cubic structures that we have considered up to this point.

We may begin to understand the diamond lattice by considering the tetrahedral structure shown in Figure 1.12. This structure is basically a body-centered cubic with four of the corner atoms missing. Every atom in the tetrahedral structure has four nearest neighbors and it is this structure that is the basic building block of the diamond lattice.
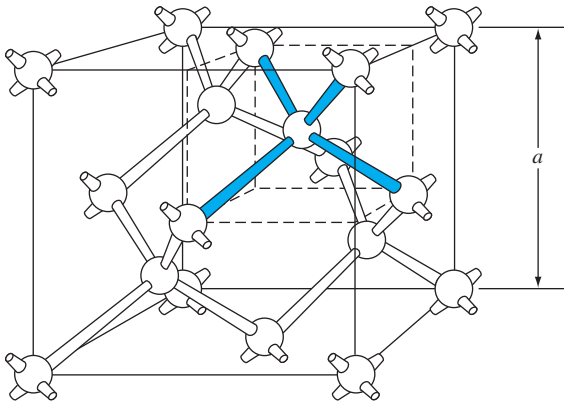
Figure 1.11 | The diamond structure.

Figure 1.12 | The tetrahedral structure of closest neighbors in the diamond lattice.
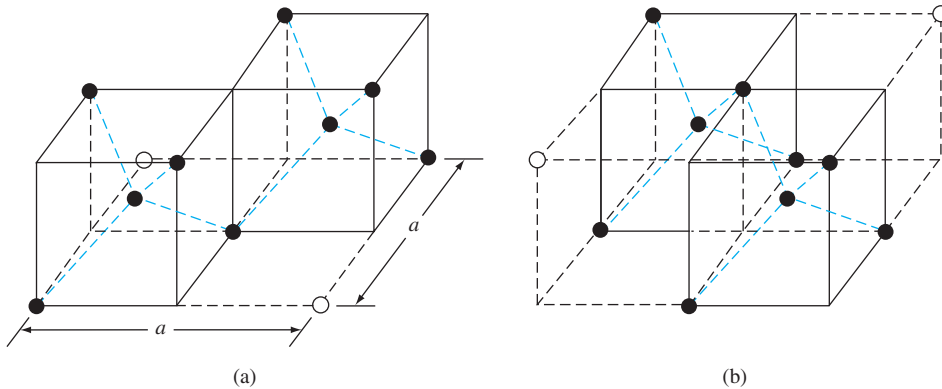
Figure 1.13 | Portions of the diamond lattice: (a) bottom half and (b) top half.

There are several ways to visualize the diamond structure. One way to gain a further understanding of the diamond lattice is by considering Figure 1.13. Figure 1.13a shows two body-centered cubic, or tetrahedral, structures diagonally adjacent to each other. The open circles represent atoms in the lattice that are generated when the structure is translated to the right or left, one lattice constant, *a*. Figure 1.13b represents the top half of the diamond structure. The top half again consists of two tetrahedral structures joined diagonally, but which are at 90° with respect to the bottom-half diagonal. An important characteristic of the diamond lattice is that any atom within the diamond structure will have four nearest neighboring atoms. We will note this characteristic again in our discussion of atomic bonding in the next section.

The diamond structure refers to the particular lattice in which all atoms are of the same species, such as silicon or germanium. The zincblende (sphalerite) structure differs from the diamond structure only in that there are two different types of atoms in the lattice. Compound semiconductors, such as gallium arsenide, have the zincblende structure shown in Figure 1.14. The important feature of both the diamond and the zincblende structures is that the atoms are joined together to form a tetrahedron. Figure 1.15 shows the basic tetrahedral structure of GaAs in which each Ga atom has four nearest As neighbors and each As atom has four nearest Ga neighbors. This figure also begins to show the interpenetration of two sublattices that can be used to generate the diamond or zincblende lattice.

## TEST YOUR UNDERSTANDING

TYU 1.4 Consider the diamond unit cell shown in Figure 1.11. Determine the (a) number of corner atoms, (b) number of face-centered atoms, and (c) number of atoms totally enclosed in the unit cell. [Ans. (a) 8; (b) 6; (c) 4]

TYU 1.5 The lattice constant of silicon is 5.43 Å. Calculate the volume density of silicon atoms. (Ans. $5 \times 10^{22} \text{ cm}^{-3}$)
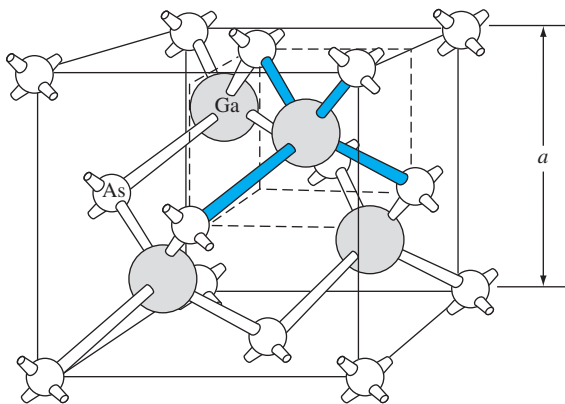
Figure 1.14 | The zincblende (sphalerite) lattice of GaAs.
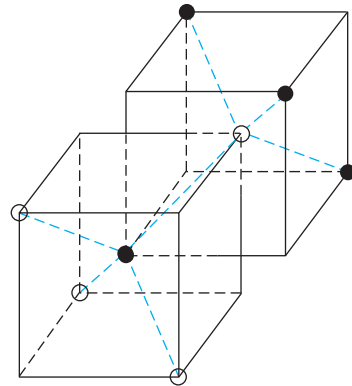
Figure 1.15 | The tetrahedral structure of closest neighbors in the zincblende lattice.
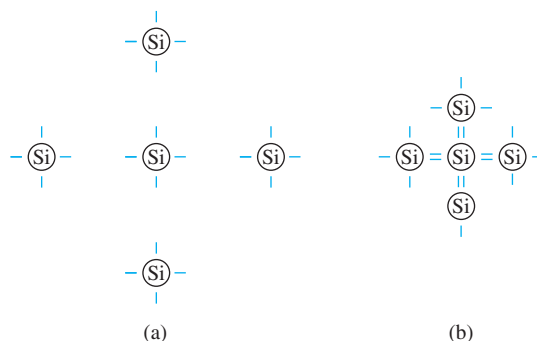
1.5 | ATOMIC BONDING

We have been considering various single-crystal structures. The question arises as to why one particular crystal structure is favored over another for a particular assembly of atoms. A fundamental law of nature is that the total energy of a system in thermal equilibrium tends to reach a minimum value. The interaction that occurs between atoms to form a solid and to reach the minimum total energy depends on the type of atom or atoms involved. The type of bond, or interaction, between atoms, then, depends on the particular atom or atoms in the crystal. If there is not a strong bond between atoms, they will not "stick together" to create a solid.

The interaction between atoms can be described by quantum mechanics. Although an introduction to quantum mechanics is presented in the next chapter, the quantum-mechanical description of the atomic bonding interaction is still beyond the scope of this text. We can nevertheless obtain a qualitative understanding of how various atoms interact by considering the valence, or outermost, electrons of an atom.

The atoms at the two extremes of the periodic table (excepting the inert elements) tend to lose or gain valence electrons, thus forming ions. These ions then essentially have complete outer energy shells. The elements in group I of the periodic table tend to lose their one electron and become positively charged, while the elements in group VII tend to gain an electron and become negatively charged. These oppositely charged ions then experience a coulomb attraction and form a bond referred to as an *ionic bond*. If the ions were to get too close, a repulsive force would become dominant, so an equilibrium distance results between these two ions. In a crystal, negatively charged ions tend to be surrounded by positively charged ions and positively charged ions tend to be surrounded by negatively charged ions, so a periodic array of the atoms is formed to create the lattice. A classic example of ionic bonding is sodium chloride.

Figure 1.16 | Representation of (a) hydrogen valence electrons and (b) covalent bonding in a hydrogen molecule.

Figure 1.17 | Representation of (a) silicon valence electrons and (b) covalent bonding in the silicon crystal.

The interaction of atoms tends to form closed valence shells such as we see in ionic bonding. Another atomic bond that tends to achieve closed-valence energy shells is *covalent bonding,* an example of which is found in the hydrogen molecule. A hydrogen atom has one electron and needs one more electron to complete the lowest energy shell. A schematic of two noninteracting hydrogen atoms, and the hydrogen molecule with the covalent bonding, is shown in Figure 1.16. Covalent bonding results in electrons being shared between atoms, so that in effect the valence energy shell of each atom is full.

Atoms in group IV of the periodic table, such as silicon and germanium, also tend to form covalent bonds. Each of these elements has four valence electrons and needs four more electrons to complete the valence energy shell. If a silicon atom, for example, has four nearest neighbors, with each neighbor atom contributing one valence electron to be shared, then the center atom will in effect have eight electrons in its outer shell. Figure 1.17a schematically shows five noninteracting silicon atoms with the four valence electrons around each atom. A two-dimensional representation of the covalent bonding in silicon is shown in Figure 1.17b. The center atom has eight shared valence electrons.

A significant difference between the covalent bonding of hydrogen and of silicon is that, when the hydrogen molecule is formed, it has no additional electrons to form additional covalent bonds, while the outer silicon atoms always have valence electrons available for additional covalent bonding. The silicon array may then be formed into an infinite crystal, with each silicon atom having four nearest neighbors and eight shared electrons. The four nearest neighbors in silicon forming the covalent bond correspond to the tetrahedral structure and the diamond lattice, which were shown in Figures 1.12 and 1.11 respectively. Atomic bonding and crystal structure are obviously directly related.

The third major atomic bonding scheme is referred to as *metallic bonding*. Group I elements have one valence electron. If two sodium atoms ($Z = 11$), for example, are brought into close proximity, the valence electrons interact in a way similar to that in covalent bonding. When a third sodium atom is brought into close proximity with the

first two, the valence electrons can also interact and continue to form a bond. Solid sodium has a body-centered cubic structure, so each atom has eight nearest neighbors with each atom sharing many valence electrons. We may think of the positive metallic ions as being surrounded by a sea of negative electrons, the solid being held together by the electrostatic forces. This description gives a qualitative picture of the metallic bond.

A fourth type of atomic bond, called the *Van der Waals* bond, is the weakest of the chemical bonds. A hydrogen fluoride (HF) molecule, for example, is formed by an ionic bond. The effective center of the positive charge of the molecule is not the same as the effective center of the negative charge. This nonsymmetry in the charge distribution results in a small electric dipole that can interact with the dipoles of other HF molecules. With these weak interactions, solids formed by the Van der Waals bonds have a relatively low melting temperature—in fact, most of these materials are in gaseous form at room temperature.

*1.6 | IMPERFECTIONS AND IMPURITIES IN SOLIDS

Up to this point, we have been considering an ideal single-crystal structure. In a real crystal, the lattice is not perfect, but contains imperfections or defects; that is, the perfect geometric periodicity is disrupted in some manner. Imperfections tend to alter the electrical properties of a material and, in some cases, electrical parameters can be dominated by these defects or impurities.

1.6.1   Imperfections in Solids

One type of imperfection that all crystals have in common is atomic thermal vibration. A perfect single crystal contains atoms at particular lattice sites, the atoms separated from each other by a distance we have assumed to be constant. The atoms in a crystal, however, have a certain thermal energy, which is a function of temperature. The thermal energy causes the atoms to vibrate in a random manner about an equilibrium lattice point. This random thermal motion causes the distance between atoms to randomly fluctuate, slightly disrupting the perfect geometric arrangement of atoms. This imperfection, called *lattice vibrations,* affects some electrical parameters, as we will see later in our discussion of semiconductor material characteristics.

Another type of defect is called a *point defect.* There are several of this type that we need to consider. Again, in an ideal single-crystal lattice, the atoms are arranged in a perfect periodic arrangement. However, in a real crystal, an atom may be missing from a particular lattice site. This defect is referred to as a *vacancy;* it is schematically shown in Figure 1.18a. In another situation, an atom may be located between lattice sites. This defect is referred to as an *interstitial* and is schematically shown in Figure 1.18b. In the case of vacancy and interstitial defects, not only is the perfect

---

*Indicates sections that will aid in the total summation of understanding of semiconductor devices, but may be skipped the first time through the text without loss of continuity.
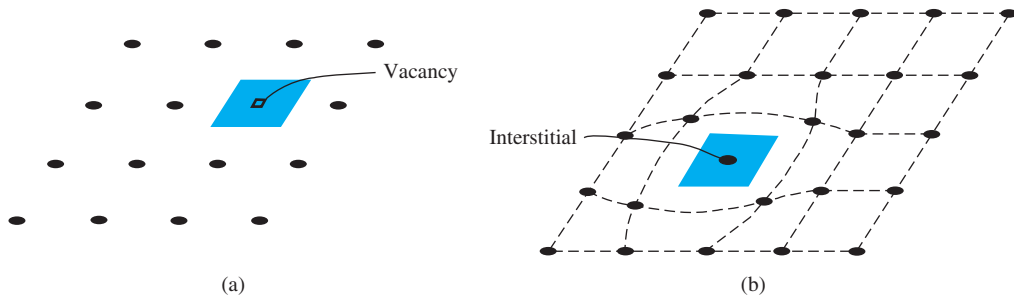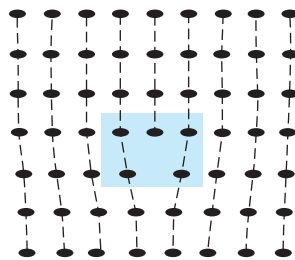
Figure 1.18 | Two-dimensional representation of a single-crystal lattice showing (a) a vacancy defect and (b) an interstitial defect.

geometric arrangement of atoms broken but also the ideal chemical bonding between atoms is disrupted, which tends to change the electrical properties of the material. A vacancy and interstitial may be in close enough proximity to exhibit an interaction between the two point defects. This vacancy–interstitial defect, also known as a *Frenkel defect,* produces different effects than the simple vacancy or interstitial.

The point defects involve single atoms or single-atom locations. In forming single-crystal materials, more complex defects may occur. A line defect, for example, occurs when an entire row of atoms is missing from its normal lattice site. This defect is referred to as a *line dislocation* and is shown in Figure 1.19. As with a point defect, a line dislocation disrupts both the normal geometric periodicity of the lattice and the ideal atomic bonds in the crystal. This dislocation can also alter the electrical properties of the material, usually in a more unpredictable manner than the simple point defects.

Other complex dislocations can also occur in a crystal lattice. However, this introductory discussion is intended only to present a few of the basic types of defect, and to show that a real crystal is not necessarily a perfect lattice structure. The effect of these imperfections on the electrical properties of a semiconductor will be considered in later chapters.

Figure 1.19 | A two-dimensional representation of a line dislocation.
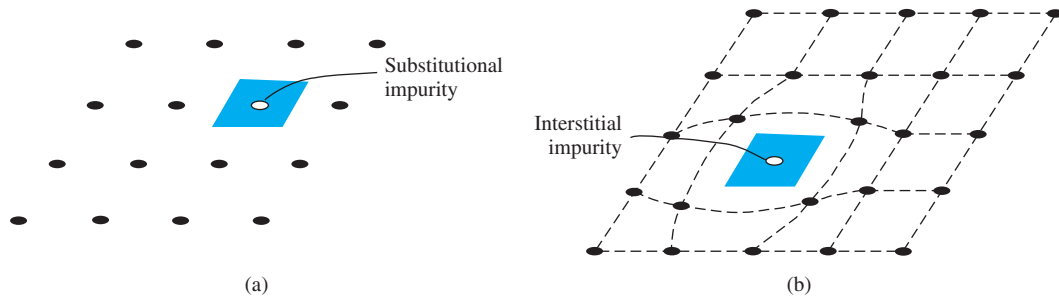
Figure 1.20 | Two-dimensional representation of a single-crystal lattice showing (a) a substitutional impurity and (b) an intersitital impurity.

1.6.2   Impurities in Solids

Foreign atoms, or impurity atoms, may be present in a crystal lattice. Impurity atoms may be located at normal lattice sites, in which case they are called *substitutional* impurities. Impurity atoms may also be located between normal sites, in which case they are called *interstitial* impurities. Both these impurities are lattice defects and are schematically shown in Figure 1.20. Some impurities, such as oxygen in silicon, tend to be essentially inert; however, other impurities, such as gold or phosphorus in silicon, can drastically alter the electrical properties of the material.

In Chapter 4 we will see that, by adding controlled amounts of particular impurity atoms, the electrical characteristics of a semiconductor material can be favorably altered. The technique of adding impurity atoms to a semiconductor material in order to change its conductivity is called *doping*. There are two general methods of doping: impurity diffusion and ion implantation.

The actual diffusion process depends to some extent on the material but, in general, impurity diffusion occurs when a semiconductor crystal is placed in a high-temperature ($\approx 1000°C$) gaseous atmosphere containing the desired impurity atom. At this high temperature, many of the crystal atoms can randomly move in and out of their single-crystal lattice sites. Vacancies may be created by this random motion so that impurity atoms can move through the lattice by hopping from one vacancy to another. Impurity diffusion is the process by which impurity particles move from a region of high concentration near the surface to a region of lower concentration within the crystal. When the temperature decreases, the impurity atoms become permanently frozen into the substitutional lattice sites. Diffusion of various impurities into selected regions of a semiconductor allows us to fabricate complex electronic circuits in a single semiconductor crystal.

Ion implantation generally takes place at a lower temperature than diffusion. A beam of impurity ions is accelerated to kinetic energies in the range of 50 keV or greater and then directed to the surface of the semiconductor. The high-energy impurity ions enter the crystal and come to rest at some average depth from the surface. One advantage of ion implantation is that controlled numbers of impurity atoms can be introduced into specific regions of the crystal. A disadvantage of this technique is that the incident impurity atoms collide with the crystal atoms, causing

lattice-displacement damage. However, most of the lattice damage can be removed by thermal annealing, in which the temperature of the crystal is raised for a short time. Thermal annealing is a required step after implantation.

*1.7 | GROWTH OF SEMICONDUCTOR MATERIALS

The success in fabricating very large scale integrated (VLSI) circuits is a result, to a large extent, of the development of and improvement in the formation or growth of pure single-crystal semiconductor materials. Semiconductors are some of the purest materials. Silicon, for example, has concentrations of most impurities of less than 1 part in 10^{10} atoms. The high purity requirement means that extreme care is necessary in the growth and the treatment of the material at each step of the fabrication process. The mechanics and kinetics of crystal growth are extremely complex and will be described in only very general terms in this text. However, a general knowledge of the growth techniques and terminology is valuable.

1.7.1   Growth from a Melt

A common technique for growing single-crystal materials is called the *Czochralski method.* In this technique, a small piece of single-crystal material, known as a *seed,* is brought into contact with the surface of the same material in liquid phase, and then slowly pulled from the melt. As the seed is slowly pulled, solidification occurs along the plane between the solid–liquid interface. Usually the crystal is also rotated slowly as it is being pulled, to provide a slight stirring action to the melt, resulting in a more uniform temperature. Controlled amounts of specific impurity atoms, such as boron or phosphorus, may be added to the melt so that the grown semiconductor crystal is intentionally doped with the impurity atom. Figure 1.21a shows a schematic of the Czochralski growth process and a silicon ingot or boule grown by this process.

   Some impurities may be present in the ingot that are undesirable. Zone refining is a common technique for purifying material. A high-temperature coil, or r-f induction coil, is slowly passed along the length of the boule. The temperature induced by the coil is high enough so that a thin layer of liquid is formed. At the solid–liquid interface, there is a distribution of impurities between the two phases. The parameter that describes this distribution is called the *segregation coefficient:* the ratio of the concentration of impurities in the solid to the concentration in the liquid. If the segregation coefficient is 0.1, for example, the concentration of impurities in the liquid is a factor of 10 greater than that in the solid. As the liquid zone moves through the material, the impurities are driven along with the liquid. After several passes of the r-f coil, most impurities are at the end of the bar, which can then be cut off. The moving molten zone, or the zone-refining technique, can result in considerable purification.

   After the semiconductor is grown, the boule is mechanically trimmed to the proper diameter and a flat is ground over the entire length of the boule to denote

---

*Indicates sections that will aid in the total summation of understanding of semiconductor devices, but may be skipped the first time through the text without loss of continuity.

(a)

(b)
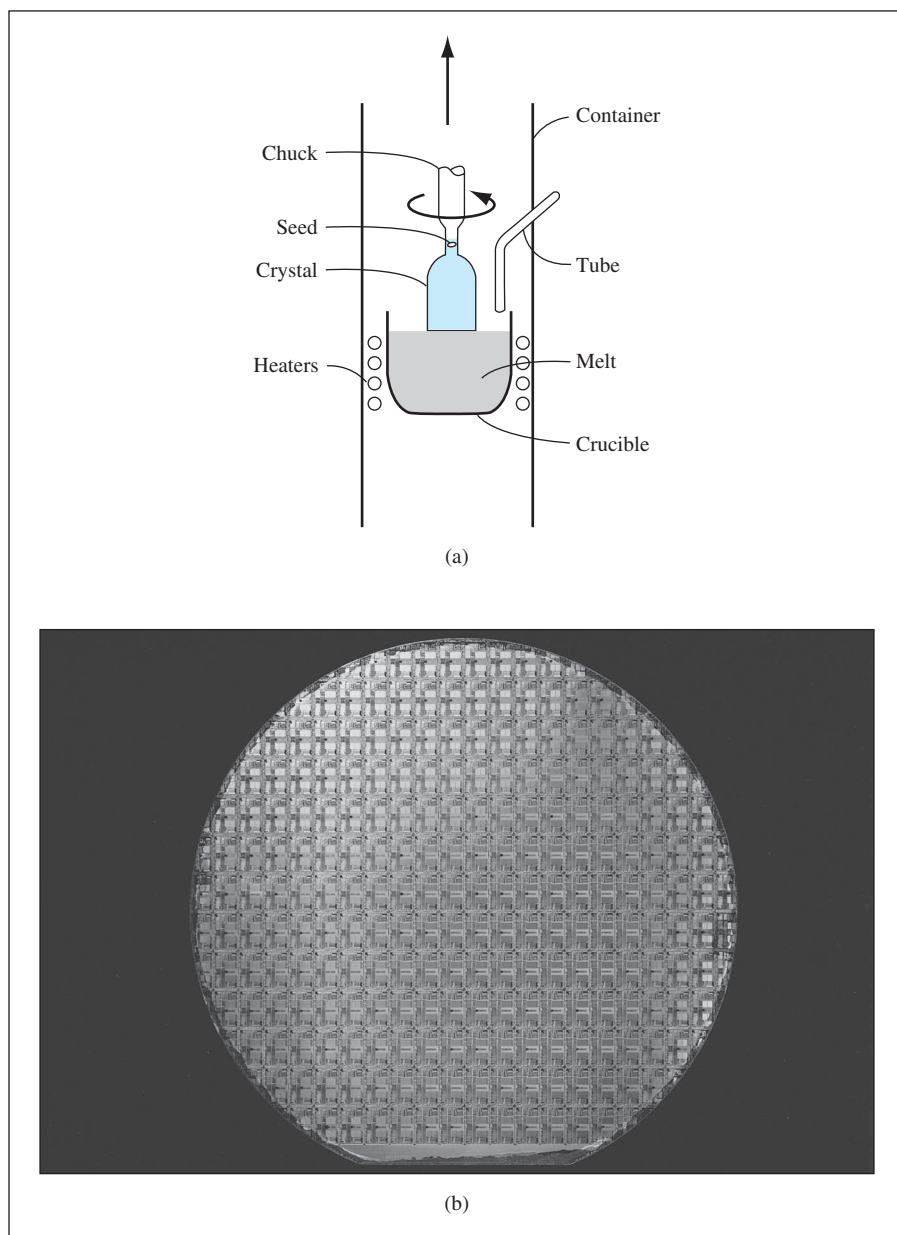
Figure 1.21 | (a) Model of a crystal puller and (b) photograph of a silicon wafer with an array of integrated circuits. The circuits are tested on the wafer then sawed apart into chips that are mounted into packages. (Photo courtesy of Intel Corporation.)

the crystal orientation. The flat is perpendicular to the [110] direction or indicates the (110) plane. (See Figure 1.21b.) This then allows the individual chips to be fabricated along given crystal planes so that the chips can be sawed apart more easily. The boule is then sliced into wafers. The wafer must be thick enough to mechanically support itself. A mechanical two-sided lapping operation produces a flat wafer of uniform thickness. Since the lapping procedure can leave a surface damaged and contaminated by the mechanical operation, the surface must be removed by chemical etching. The final step is polishing. This provides a smooth surface on which devices may be fabricated or further growth processes may be carried out. This final semiconductor wafer is called the substrate material.

1.7.2 Epitaxial Growth

A common and versatile growth technique that is used extensively in device and integrated circuit fabrication is epitaxial growth. *Epitaxial growth* is a process whereby a thin, single-crystal layer of material is grown on the surface of a single-crystal substrate. In the epitaxial process, the single-crystal substrate acts as the seed, although the process takes place far below the melting temperature. When an epitaxial layer is grown on a substrate of the same material, the process is termed *homoepitaxy.* Growing silicon on a silicon substrate is one example of a homoepitaxy process. At present, a great deal of work is being done with *heteroepitaxy.* In a heteroepitaxy process, although the substrate and epitaxial materials are not the same, the two crystal structures should be very similar if single-crystal growth is to be obtained and if a large number of defects are to be avoided at the epitaxial–substrate interface. Growing epitaxial layers of the ternary alloy AlGaAs on a GaAs substrate is one example of a heteroepitaxy process.

One epitaxial growth technique that has been used extensively is called *chemical vapor-phase deposition* (CVD). Silicon epitaxial layers, for example, are grown on silicon substrates by the controlled deposition of silicon atoms onto the surface from a chemical vapor containing silicon. In one method, silicon tetrachloride reacts with hydrogen at the surface of a heated substrate. The silicon atoms are released in the reaction and can be deposited onto the substrate, while the other chemical reactant, HCl, is in gaseous form and is swept out of the reactor. A sharp demarcation between the impurity doping in the substrate and in the epitaxial layer can be achieved using the CVD process. This technique allows great flexibility in the fabrication of semiconductor devices.

Liquid-phase epitaxy is another epitaxial growth technique. A compound of the semiconductor with another element may have a melting temperature lower than that of the semiconductor itself. The semiconductor substrate is held in the liquid compound and, since the temperature of the melt is lower than the melting temperature of the substrate, the substrate does not melt. As the solution is slowly cooled, a single-crystal semiconductor layer grows on the seed crystal. This technique, which occurs at a lower temperature than the Czochralski method, is useful in growing group III–V compound semiconductors.

A versatile technique for growing epitaxial layers is the *molecular beam epitaxy* (MBE) process. A substrate is held in vacuum at a temperature normally in the range

of 400 to 800°C, a relatively low temperature compared with many semiconductor-processing steps. Semiconductor and dopant atoms are then evaporated onto the surface of the substrate. In this technique, the doping can be precisely controlled resulting in very complex doping profiles. Complex ternary compounds, such as AlGaAs, can be grown on substrates, such as GaAs, where abrupt changes in the crystal composition are desired. Many layers of various types of epitaxial compositions can be grown on a substrate in this manner. These structures are extremely beneficial in optical devices such as laser diodes.

1.8 | SUMMARY

■ A few of the most common semiconductor materials were listed. Silicon is the most common semiconductor material and appears in column IV of the periodic table.

■ The properties of semiconductors and other materials are determined to a large extent by the single-crystal lattice structure. The unit cell is a small volume of the crystal that is used to reproduce the entire crystal. Three basic unit cells are the simple cubic, body-centered cubic, and face-centered cubic.

■ Silicon has the diamond crystal structure. Atoms are formed in a tetrahedral configuration with four nearest neighbor atoms. The binary semiconductors have a zincblende lattice that is basically the same as the diamond lattice.

■ Miller indices are used to describe planes in a crystal lattice. These planes may be used to describe the surface of a semiconductor material. The Miller indices are also used to describe directions in a crystal.

■ Imperfections do exist in semiconductor materials. A few of these imperfections are vacancies, substitutional impurities, and interstitial impurities. Small amounts of controlled substitutional impurities can favorably alter semiconductor properties as we will see in later chapters.

■ A brief description of semiconductor growth methods was given. Bulk growth, such as the Czochralski method, produces the starting semiconductor material or substrate. Epitaxial growth can be used to control the surface properties of a semiconductor. Most semiconductor devices are fabricated in the epitaxial layer.

GLOSSARY OF IMPORTANT TERMS

binary semiconductor   A two-element compound semiconductor, such as gallium arsenide (GaAs).

covalent bonding   The bonding between atoms in which valence electrons are shared.

diamond lattice   The atomic crystal structure of silicon, for example, in which each atom has four nearest neighbors in a tetrahedral configuration.

doping   The process of adding specific types of atoms to a semiconductor to favorably alter the electrical characteristics.

elemental semiconductor   A semiconductor composed of a single species of atom, such as silicon or germanium.

epitaxial layer   A thin, single-crystal layer of material formed on the surface of a substrate.

ion implantation   One particular process of doping a semiconductor.

lattice   The periodic arrangement of atoms in a crystal.

Miller indices   The set of integers used to describe a crystal plane.

primitive cell   The smallest unit cell that can be repeated to form a lattice.

substrate   A semiconductor wafer or other material used as the starting material for further semiconductor processing, such as epitaxial growth or diffusion.

ternary semiconductor   A three-element compound semiconductor, such as aluminum gallium arsenide (AlGaAs).

unit cell   A small volume of a crystal that can be used to reproduce the entire crystal.

zincblende lattice   A lattice structure identical to the diamond lattice except that there are two types of atoms instead of one.

CHECKPOINT

After studying this chapter, the reader should have the ability to:

■   List the most common elemental semiconductor material.
■   Describe the concept of a unit cell.
■   Determine the volume density of atoms for various lattice structures.
■   Determine the Miller indices of a crystal-lattice plane.
■   Sketch a lattice plane given the Miller indices.
■   Determine the surface density of atoms on a given crystal-lattice plane.
■   Describe the tetrahedral configuration of silicon atoms.
■   Understand and describe various defects in a single-crystal lattice.

REVIEW QUESTIONS

1.   List two elemental semiconductor materials and two compound semiconductor materials.

2.   Sketch three lattice structures: (*a*) simple cubic, (*b*) body-centered cubic, and (*c*) face-centered cubic.

3.   Describe the procedure for finding the volume density of atoms in a crystal.

4.   Describe the procedure for obtaining the Miller indices that describe a plane in a crystal.

5.   Describe the procedure for finding the surface density of atoms on a particular lattice plane.

6.   Describe why a unit cell, that is not a primitive unit cell, might be preferable to a primitive unit cell.

7.   Describe covalent bonding in silicon.

8.   What is meant by a substitutional impurity in a crystal? What is meant by an interstitial impurity?

PROBLEMS

Section 1.3   Space Lattices

1.1   Determine the number of atoms per unit cell in a (*a*) face-centered cubic, (*b*) body-centered cubic, and (*c*) diamond lattice.

1.2   Assume that each atom is a hard sphere with the surface of each atom in contact with the surface of its nearest neighbor. Determine the percentage of total unit cell volume