

Fourth Edition

PRINCIPLES OF  
**Electronic  
Materials  
& Devices**



**Mc  
Graw  
Hill**  
Education

S. O. KASAP

# PRINCIPLES OF ELECTRONIC MATERIALS AND DEVICES

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**FOURTH EDITION**

**S. O. Kasap**

*University of Saskatchewan  
Canada*

**Mc  
Graw  
Hill**  
Education



## PRINCIPLES OF ELECTRONIC MATERIALS AND DEVICES, FOURTH EDITION

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Paul Dirac (1902–1984) and Werner Heisenberg (1901–1976) walking outdoors in Cambridge circa 1930. They received the Nobel Prize in Physics in 1928 and 1932, respectively.

| Courtesy of AIP Emilio Segre Visual Archives, Physics Today Collection



Max Planck (1858–1947), a German theoretical physicist, was one of the originators of quantum theory, and won the Nobel Prize in Physics in 1918. His Nobel citation is “*in recognition of the services he rendered to the advancement of Physics by his discovery of energy quanta*”.

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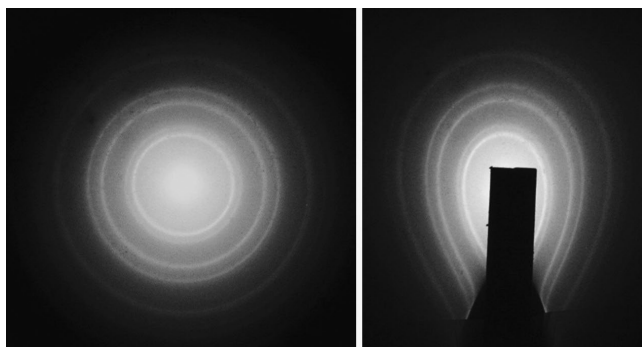
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Left: Circular bright rings make up the diffraction pattern obtained when an electron beam is passed through a thin polycrystalline aluminum sheet. The pattern results from the wave behavior of the electrons; the waves are diffracted by the Al crystals. Right: A magnet brought to the screen bends the electron paths and distorts the diffraction pattern. The magnet would have no effect if the pattern was due to X-rays, which are electromagnetic waves. Courtesy of Farley Chicilo

# PREFACE

## FOURTH EDITION

The textbook represents a first course in electronic materials and devices for undergraduate students. With the additional topics, the text can also be used in a graduate-level introductory course in electronic materials for electrical engineers and material scientists. The fourth edition is an extensively revised and extended version of the third edition based on reviewer comments and the developments in electronic and optoelectronic materials over the last ten years. The fourth edition has many new and expanded topics, new worked examples, new illustrations, and new homework problems. The majority of the illustrations have been greatly improved to make them clearer. A very large number of new homework problems have been added, and many more solved problems have been provided that put the concepts into applications. More than 50% of the illustrations have gone through some kind of revision to improve the clarity. Furthermore, more terms have been added under *Defining Terms*, which the students have found very useful. Bragg's diffraction law that is mentioned in several chapters is kept as Appendix A for those readers who are unfamiliar with it.

The fourth edition is one of the few books on the market that have a broad coverage of electronic materials that today's scientists and engineers need. I believe that the revisions have improved the rigor without sacrificing the original semiquantitative approach that both the students and instructors liked. The major revisions in scientific content can be summarized as follows:

Chapter 1 Thermal expansion; kinetic molecular theory; atomic diffusion; molecular collisions and vacuum deposition; particle flux density;

line defects; planar defects; crystal surfaces; Grüneisen's rule.

Chapter 2 Temperature dependence of resistivity, strain gauges, Hall effect; ionic conduction; Einstein relation for drift mobility and diffusion; ac conductivity; resistivity of thin films; interconnects in microelectronics; electromigration.

Chapter 3 Electron as a wave; infinite potential well; confined electron in a finite potential energy well; stimulated emission and photon amplification; He-Ne laser, optical fiber amplification.

Chapter 4 Work function; electron photoemission; secondary emission; electron affinity and photomultiplication; Fermi-Dirac statistics; conduction in metals; thermoelectricity and Seebeck coefficient; thermocouples; phonon concentration changes with temperature.

Chapter 5 Degenerate semiconductors; direct and indirect recombination;  $E$  vs.  $k$  diagrams for direct and indirect bandgap semiconductors; Schottky junction and depletion layer; Seebeck effect in semiconductors and voltage drift.

Chapter 6 The  $pn$  junction; direct bandgap  $pn$  junction; depletion layer capacitance; linearly graded junction; hyperabrupt junctions; light emitting diodes (LEDs); quantum well high intensity LEDs; LED materials and structures; LED characteristics; LED spectrum; brightness



	and efficiency of LEDs; multi-junction solar cells.
Chapter 7	Atomic polarizability; interfacial polarization; impact ionization in gases and breakdown; supercapacitors.
Chapter 8	anisotropic and giant magnetoresistance; magnetic recording materials; longitudinal and vertical magnetic recording; materials for magnetic storage; superconductivity.
Chapter 9	Refractive and group index of Si; dielectric mirrors; free carrier absorption; liquid crystal displays.

## ORGANIZATION AND FEATURES

In preparing the fourth edition, as in previous edition, I tried to keep the general treatment and various proofs at a semiquantitative level without going into detailed physics. Many of the problems have been set to satisfy engineering accreditation requirements. Some chapters in the text have additional topics to allow a more detailed treatment, usually including quantum mechanics or more mathematics. Cross referencing has been avoided as much as possible without too much repetition and to allow various sections and chapters to be skipped as desired by the reader. The text has been written so as to be easily usable in one-semester courses by allowing such flexibility.

Some important features are:

- The principles are developed with the minimum of mathematics and with the emphasis on physical ideas. Quantum mechanics is part of the course but without its difficult mathematical formalism.
- There are numerous worked examples or solved problems, most of which have a practical significance. Students learn by way of examples, however simple, and to that end a large number (227 in total) of solved problems have been provided.

- Even simple concepts have examples to aid learning.
- Most students would like to have clear diagrams to help them visualize the explanations and understand concepts. The text includes 565 illustrations that have been professionally prepared to reflect the concepts and aid the explanations in the text. There are also numerous photographs of practical devices and scientists and engineers to enhance the learning experience.
- The end-of-chapter questions and problems (346 in total) are graded so that they start with easy concepts and eventually lead to more sophisticated concepts. Difficult problems are identified with an asterisk (\*). Many practical applications with diagrams have been included.
- There is a glossary, *Defining Terms*, at the end of each chapter that defines some of the concepts and terms used, not only within the text but also in the problems.
- The end of each chapter includes a section *Additional Topics* to further develop important concepts, to introduce interesting applications, or to prove a theorem. These topics are intended for the keen student and can be used as part of the text for a two-semester course.
- The text is supported by McGraw-Hill's textbook website that contains resources, such as solved problems, for both students and instructors.
- The fourth edition is supported by an extensive PowerPoint presentation for instructors who have adopted the book for their course. The PowerPoint has all the illustrations in color, and includes additional color photos. The basic concepts and equations are also highlighted in additional slides.
- There is a regularly updated online extended *Solutions Manual* for all instructors; simply locate the McGraw-Hill website for this textbook. The Solutions Manual provides not only detailed explanations to the solutions, but also has color diagrams as well as

references and helpful notes for instructors. (It also has the answers to those “why?” questions in the text.)

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My gratitude goes to my past and present graduate students and postdoctoral research fellows, who have kept me on my toes and read various sections of this book. I have been fortunate to have a colleague and friend like Charbel Tannous (Brest University) who, as usual, made many sharply critical but helpful comments, especially on Chapter 8. My best friend and colleague of many years Robert Johanson (University of Saskatchewan), with whom I share teaching this course, also provided a number of critical comments towards the fourth edition. A number of reviewers, at various times, read various portions of the manuscript and provided extensive comments. A number of instructors also wrote to me with their own comments. I incorporated the majority of the suggestions, which I believe made this a better book. No textbook is perfect, and I’m sure that there will be more suggestions (and corrections) for the next edition. I’d like to personally thank them all for their invaluable critiques.

I’d like to thank Tina Bower, my present Product Developer, and Raghu Srinivasan, my

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**Safa Kasap**

Saskatoon, March, 2017

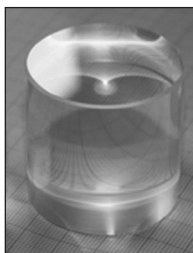
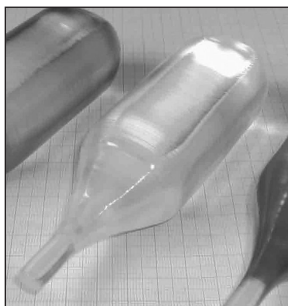
“The important thing in science is not so much to obtain new facts as to discover new ways of thinking about them.”

*Sir William Lawrence Bragg*



Left: GaAs ingots and wafers. GaAs is a III-V compound semiconductor because Ga and As are from Groups III and V, respectively. Right: An  $\text{In}_x\text{Ga}_{1-x}\text{As}$  (a III-V compound semiconductor)-based photodetector.

Left: Courtesy of Sumitomo Electric Industries. Right: Courtesy of Thorlabs.



Left: A detector structure that will be used to detect dark matter particles. Each individual cylindrical detector has a  $\text{CaWO}_4$  single crystal, similar to that shown on the bottom right. These crystals are called scintillators, and convert high-energy radiation to light. The Czochralski technique is used to grow the crystal shown on top right, which is a  $\text{CaWO}_4$  ingot. The detector crystal is cut from this ingot.

Left: Courtesy of Max Planck Institute for Physics. Right: Reproduced from Andreas Erb and Jean-Come Lanfranchi, *CrystEngCom*, 15, 2301, 2015, by permission of the Royal Society of Chemistry. All rights reserved.

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## CHAPTER

# 1

## Elementary Materials Science Concepts<sup>1</sup>

Understanding the basic building blocks of matter has been one of the most intriguing endeavors of humankind. Our understanding of interatomic interactions has now reached a point where we can quite comfortably explain the macroscopic properties of matter, based on quantum mechanics and electrostatic interactions between electrons and ionic nuclei in the material. There are many properties of materials that can be explained by a classical treatment of the subject. In this chapter, as well as in Chapter 2, we treat the interactions in a material from a classical perspective and introduce a number of elementary concepts. These concepts do not invoke any quantum mechanics, which is a subject of modern physics and is introduced in Chapter 3. Although many useful engineering properties of materials can be treated with hardly any quantum mechanics, it is impossible to develop the science of electronic materials and devices without modern physics.

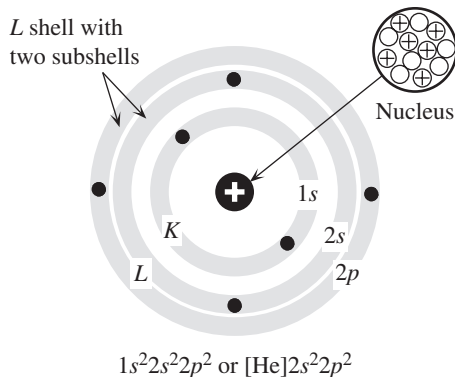
### 1.1 ATOMIC STRUCTURE AND ATOMIC NUMBER

The model of the atom that we must use to understand the atom's general behavior involves quantum mechanics, a topic we will study in detail in Chapter 3. For the present, we will simply accept the following facts about a simplified, but intuitively satisfactory, atomic model called the **shell model**, based on the **Bohr model** (1913).

The mass of the atom is concentrated at the nucleus, which contains protons and neutrons. Protons are positively charged particles, whereas neutrons are neutral particles, and both have about the same mass. Although there is a Coulombic repulsion

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<sup>1</sup> This chapter may be skipped by readers who have already been exposed to an elementary course in materials science.



**Figure 1.1** The shell model of the carbon atom, in which the electrons are confined to certain shells and subshells within shells.

between the protons, all the protons and neutrons are held together in the nucleus by the **strong force**, which is a powerful, fundamental, natural force between particles. This force has a very short range of influence, typically less than  $10^{-15}$  m. When the protons and neutrons are brought together very closely, the strong force overcomes the electrostatic repulsion between the protons and keeps the nucleus intact. The number of protons in the nucleus is the **atomic number**  $Z$  of the element.

The electrons are assumed to be orbiting the nucleus at very large distances compared to the size of the nucleus. There are as many orbiting electrons as there are protons in the nucleus. An important assumption in the Bohr model is that only certain orbits with fixed radii are stable around the nucleus. For example, the closest orbit of the electron in the hydrogen atom can only have a radius of 0.053 nm. Since the electron is constantly moving around an orbit with a given radius, over a long time period (perhaps  $\sim 10^{-12}$  seconds on the atomic time scale), the electron would appear as a spherical negative-charge cloud around the nucleus and not as a single dot representing a finite particle. We can therefore view the electron as a charge contained within a spherical **shell** of a given radius.

Due to the requirement of stable orbits, the electrons therefore do not randomly occupy the whole region around the nucleus. Instead, they occupy various well-defined spherical regions. They are distributed in various shells and **subshells** within the shells, obeying certain occupation (or seating) rules.<sup>2</sup> The example for the carbon atom is shown in Figure 1.1.

The shells and subshells that define the whereabouts of the electrons are labeled using two sets of integers,  $n$  and  $\ell$ . These integers are called the **principal** and **orbital angular momentum quantum numbers**, respectively. (The meanings of these names are not critical at this point.) The integers  $n$  and  $\ell$  have the values  $n = 1, 2, 3, \dots$ , and  $\ell = 0, 1, 2, \dots, n - 1$ , and  $\ell < n$ . For each choice of  $n$ , there are  $n$  values of  $\ell$ , so higher-order shells contain more subshells. The shells corresponding to  $n = 1, 2, 3, 4, \dots$  are labeled by the capital letters  $K, L, M, N, \dots$ , and the subshells denoted by  $\ell = 0, 1, 2, 3, \dots$  are labeled  $s, p, d, f, \dots$ . The

<sup>2</sup> In Chapter 3, in which we discuss the quantum mechanical model of the atom, we will see that these shells and subshells are spatial regions around the nucleus where the electrons are most likely to be found.



**Table 1.1** Maximum possible number of electrons in the shells and subshells of an atom

<i>n</i>	Shell	Subshell			
		$\ell = 0$ <i>s</i>	<b>1</b> <i>p</i>	<b>2</b> <i>d</i>	<b>3</b> <i>f</i>
1	<i>K</i>	2			
2	<i>L</i>	2	6		
3	<i>M</i>	2	6	10	
4	<i>N</i>	2	6	10	14

subshell with  $\ell = 1$  in the  $n = 2$  shell is thus labeled the  $2p$  subshell, based on the standard notation  $n\ell$ .

There is a definite rule to filling up the subshells with electrons; we cannot simply put all the electrons in one subshell. The number of electrons a given subshell can take is fixed by nature to be<sup>3</sup>  $2(2\ell + 1)$ . For the  $s$  subshell ( $\ell = 0$ ), there are two electrons, whereas for the  $p$  subshell, there are six electrons, and so on. Table 1.1 summarizes the most number of electrons that can be put into various subshells and shells of an atom. Obviously, the larger the shell, the more electrons it can take, simply because it contains more subshells. The shells and subshells are filled starting with those closest to the nucleus as explained next.

The number of electrons in a subshell is indicated by a superscript on the subshell symbol, so the electronic structure, or configuration, of the carbon atom (atomic number 6) shown in Figure 1.1 becomes  $1s^2 2s^2 2p^2$ . The *K* shell has only one subshell, which is full with two electrons. This is the structure of the inert element He. We can therefore write the electronic configuration more simply as  $[\text{He}]2s^2 2p^2$ . The general rule is to put the nearest previous inert element, in this case He, in square brackets and write the subshells thereafter.

The electrons occupying the outer subshells are the farthest away from the nucleus and have the most important role in atomic interactions, as in chemical reactions, because these electrons are the first to interact with outer electrons on neighboring atoms. The outermost electrons are called **valence electrons** and they determine the **valency** of the atom. Figure 1.1 shows that carbon has four valence electrons in the *L* shell.

When a subshell is full of electrons, it cannot accept any more electrons and it is said to have acquired a stable configuration. This is the case with the inert elements at the right-hand side of the Periodic Table, all of which have completely filled subshells and are rarely involved in chemical reactions. The majority of such elements are gases inasmuch as the atoms do not bond together easily to form a liquid or solid. They are sometimes used to provide an inert atmosphere instead of air for certain reactive materials.

<sup>3</sup> We will actually show this in Chapter 3 using quantum mechanics.

In an atom such as the Li atom, there are two electrons in the  $1s$  subshell and one electron in the  $2s$  subshell. The atomic structure of Li is  $1s^2 2s^1$ . The third electron is in the  $2s$  subshell, rather than any other subshell, because this is the arrangement of the electrons that results in the lowest overall energy for the whole atom. It requires energy (work) to take the third electron from the  $2s$  to the  $2p$  or higher subshells as will be shown in Chapter 3. Normally the zero energy reference corresponds to the electron being at infinity, that is, isolated from the atom. When the electron is inside the atom, its energy is negative, which is due to the attraction of the positive nucleus. An electron that is closer to the nucleus has a lower energy. The electrons nearer the nucleus are more closely bound and have higher binding energies. The  $1s^2 2s^1$  configuration of electrons corresponds to the lowest energy structure for Li and, at the same time, obeys the occupation rules for the subshells. If the  $2s$  electron is somehow excited to another outer subshell, the energy of the atom increases, and the atom is said to be **excited**.

The smallest energy required to remove a single electron from a neutral atom and thereby create a positive ion (*cation*) and an isolated electron is defined as the **ionization energy** of the atom. The Na atom has only a single valence electron in its outer shell, which is the easiest to remove. The energy required to remove this electron is 5.1 electron volts (eV), which is the Na atom's ionization energy. The **electron affinity** represents the energy that is needed, or released, when we add an electron to a neutral atom to create a negative ion (*anion*). Notice that the ionization term implies the generation of a positive ion, whereas the electron affinity implies that we have created a negative ion. Certain atoms, notably the halogens (such as F, Cl, Br, and I), can actually attract an electron to form a negative ion. Their electron affinities are negative. When we place an electron into a Cl atom, we find that an energy of 3.6 eV is *released*. The  $\text{Cl}^-$  ion has a lower energy than the Cl atom, which means that it is energetically favorable to form a  $\text{Cl}^-$  ion by introducing an electron into the Cl atom.

There is a very useful theorem in physics, called the **Virial theorem**, that allows us to relate the average kinetic energy  $\overline{KE}$ , average potential energy  $\overline{PE}$ , and average total or overall energy  $\overline{E}$  of an electron in an atom, or electrons and nuclei in a molecule, through two remarkably simple relationships,<sup>4</sup>

Virial  
theorem

$$\overline{E} = \overline{KE} + \overline{PE} \quad \text{and} \quad \overline{KE} = -\frac{1}{2}\overline{PE} \quad [1.1]$$

For example, if we define zero energy for the H atom as the  $\text{H}^+$  ion and the electron infinitely separated, then the energy of the electron in the H atom is  $-13.6$  eV. It takes 13.6 eV to ionize the H atom. The average  $\overline{PE}$  of the electron, due to its Coulombic interaction with the positive nucleus, is  $-27.2$  eV. Its average  $\overline{KE}$  turns out to be 13.6 eV. Example 1.1 uses the Virial theorem to calculate the radius of the hydrogen atom, the velocity of the electron, and its frequency of rotation.

<sup>4</sup> While the final result stated in Equation 1.1 is elegantly simple, the actual proof is quite involved and certainly not trivial. As stated here, the Virial theorem applies to a system of charges that interact through electrostatic forces only.

**VIRIAL THEOREM AND THE BOHR ATOM** Consider the hydrogen atom in Figure 1.2 in which the electron is in the stable  $1s$  orbit with a radius  $r_o$ . The ionization energy of the hydrogen atom is 13.6 eV.

**EXAMPLE 1.1**

- It takes 13.6 eV to ionize the hydrogen atom, *i.e.*, to remove the electron to infinity. If the condition when the electron is far removed from the hydrogen nucleus defines the zero reference of energy, then the total energy of the electron within the H atom is  $-13.6$  eV. Calculate the average  $PE$  and average  $KE$  of the electron.
- Assume that the electron is in a stable orbit of radius  $r_o$  around the positive nucleus. What is the Coulombic  $PE$  of the electron? Hence, what is the radius  $r_o$  of the electron orbit?
- What is the velocity of the electron?
- What is the frequency of rotation (oscillation) of the electron around the nucleus?

**SOLUTION**

- a. From Equation 1.1 we obtain

$$\bar{E} = \bar{PE} + \bar{KE} = \frac{1}{2}\bar{PE}$$

or 
$$\bar{PE} = 2\bar{E} = 2 \times (-13.6 \text{ eV}) = -27.2 \text{ eV}$$

The average kinetic energy is

$$\bar{KE} = -\frac{1}{2}\bar{PE} = 13.6 \text{ eV}$$

- b. The Coulombic  $PE$  of interaction between two charges  $Q_1$  and  $Q_2$  separated by a distance  $r_o$ , from elementary electrostatics, is given by

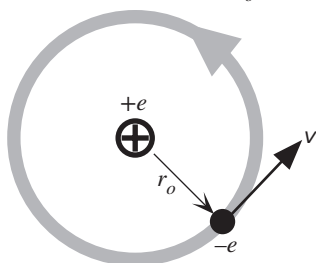
$$PE = \frac{Q_1 Q_2}{4\pi\epsilon_o r_o} = \frac{(-e)(+e)}{4\pi\epsilon_o r_o} = -\frac{e^2}{4\pi\epsilon_o r_o}$$

where we substituted  $Q_1 = -e$  (electron's charge), and  $Q_2 = +e$  (charge of the nucleus). Thus the radius  $r_o$  is

$$\begin{aligned} r_o &= -\frac{(1.6 \times 10^{-19} \text{ C})^2}{4\pi(8.85 \times 10^{-12} \text{ F m}^{-1})(-27.2 \text{ eV} \times 1.6 \times 10^{-19} \text{ J/eV})} \\ &= 5.29 \times 10^{-11} \text{ m} \quad \text{or} \quad 0.0529 \text{ nm} \end{aligned}$$

which is called the **Bohr radius** (also denoted  $a_o$ ).

Stable orbit has radius  $r_o$



**Figure 1.2** The planetary model of the hydrogen atom in which the negatively charged electron orbits the positively charged nucleus.

c. Since  $KE = \frac{1}{2}m_e v^2$ , the average velocity is

$$v = \sqrt{\frac{KE}{\frac{1}{2}m_e}} = \sqrt{\frac{13.6 \text{ eV} \times 1.6 \times 10^{-19} \text{ J/eV}}{\frac{1}{2}(9.1 \times 10^{-31} \text{ kg})}} = 2.19 \times 10^6 \text{ m s}^{-1}$$

d. The period of orbital rotation  $T$  is

$$T = \frac{2\pi r_o}{v} = \frac{2\pi(0.0529 \times 10^{-9} \text{ m})}{2.19 \times 10^6 \text{ m s}^{-1}} = 1.52 \times 10^{-16} \text{ seconds}$$

The orbital frequency  $f = 1/T = 6.59 \times 10^{15} \text{ s}^{-1}$  (Hz).

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## 1.2 ATOMIC MASS AND MOLE

We had defined the atomic number  $Z$  as the number of protons in the nucleus of an atom. The **atomic mass number**  $A$  is simply the total number of protons and neutrons in the nucleus. It may be thought that we can use the atomic mass number  $A$  of an atom to gauge its atomic mass, but this is done slightly differently to account for the existence of different isotopes of an element; isotopes are atoms of a given element that have the same number of protons but a different number of neutrons in the nucleus. The **atomic mass unit** (amu)  $u$  is a convenient atomic mass unit that is equal to  $\frac{1}{12}$  of the mass of a neutral carbon atom that has a mass number  $A = 12$  (6 protons and 6 neutrons). It has been found that  $u = 1.66054 \times 10^{-27} \text{ kg}$ .

The **atomic mass** or **relative atomic mass** or simply **atomic weight**  $M_{\text{at}}$  of an element is the average atomic mass, in atomic mass units, of all the naturally occurring isotopes of the element. Atomic masses are listed in the Periodic Table. **Avogadro's number**  $N_A$  is the number of atoms in exactly 12 grams of carbon-12, which is  $6.022 \times 10^{23}$  to three decimal places. Since the atomic mass  $M_{\text{at}}$  is defined as  $\frac{1}{12}$  of the mass of the carbon-12 atom, it is straightforward to show that  $N_A$  number of atoms of any substance have a mass equal to the atomic mass  $M_{\text{at}}$  in grams.

A **mole** of a substance is that amount of the substance that contains exactly Avogadro's number  $N_A$  of atoms or molecules that make up the substance. One mole of a substance has a mass as much as its atomic (molecular) mass in grams. For example, 1 mole of copper contains  $6.022 \times 10^{23}$  number of copper atoms and has a mass of 63.55 grams. Thus, an amount of an element that has  $6.022 \times 10^{23}$  atoms has a mass in grams equal to the atomic mass. This means we can express the atomic mass as grams per unit mole ( $\text{g mol}^{-1}$ ). The atomic mass of Au is 196.97 amu or  $\text{g mol}^{-1}$ . Thus, a 10 gram bar of gold has  $(10 \text{ g})/(196.97 \text{ g mol}^{-1})$  or 0.0507 moles.

Frequently we have to convert the composition of a substance from atomic percentage to weight percentage, and vice versa. Compositions in materials engineering generally use weight percentages, whereas chemical formulas are given in terms of atomic composition. Suppose that a substance (an alloy or a compound) is composed of two elements, A and B. Let the *weight fractions* of A and B be  $w_A$  and  $w_B$ , respectively. Let  $n_A$  and  $n_B$  be the *atomic* or *molar fractions* of A and B; that is,  $n_A$  represents the fraction of type A atoms,  $n_B$  represents the fraction of type B atoms

in the whole substance, and  $n_A + n_B = 1$ . Suppose that the atomic masses of A and B are  $M_A$  and  $M_B$ . Then  $n_A$  and  $n_B$  are given by

$$n_A = \frac{w_A/M_A}{w_A/M_A + w_B/M_B} \quad \text{and} \quad n_B = 1 - n_A \quad [1.2]$$

*Weight to atomic percentage*

where  $w_A + w_B = 1$ . Equation 1.2 can be readily rearranged to obtain  $w_A$  and  $w_B$  in terms of  $n_A$  and  $n_B$ .

**COMPOSITIONS IN ATOMIC AND WEIGHT PERCENTAGES** Consider a Pb–Sn solder that is 38.1 wt.% Pb and 61.9 wt.% Sn (this is the eutectic composition with the lowest melting point). What are the atomic fractions of Pb and Sn in this solder?

**EXAMPLE 1.2**

**SOLUTION**

For Pb, the weight fraction and atomic mass are, respectively,  $w_A = 0.381$  and  $M_A = 207.2 \text{ g mol}^{-1}$  and for Sn,  $w_B = 0.619$  and  $M_B = 118.71 \text{ g mol}^{-1}$ . Thus, Equation 1.2 gives

$$n_A = \frac{w_A/M_A}{w_A/M_A + w_B/M_B} = \frac{(0.381)/(207.2)}{0.381/207.2 + 0.619/118.71} = 0.261 \quad \text{or} \quad 26.1 \text{ at.}\%$$

and

$$n_B = \frac{w_B/M_B}{w_A/M_A + w_B/M_B} = \frac{(0.619)/(118.71)}{0.381/207.2 + 0.619/118.71} = 0.739 \quad \text{or} \quad 73.9 \text{ at.}\%$$

Thus the alloy is 26.1 at.% Pb and 73.9 at.% Sn, which can be written as  $\text{Pb}_{0.261} \text{Sn}_{0.739}$ .

## 1.3 BONDING AND TYPES OF SOLIDS

### 1.3.1 MOLECULES AND GENERAL BONDING PRINCIPLES

When two atoms are brought together, the valence electrons interact with each other and with the neighbor's positively charged nucleus. The result of this interaction is often the formation of a bond between the two atoms, producing a molecule. The formation of a bond means that the energy of the system of two atoms together must be less than that of the two atoms separated, so that the molecule formation is energetically favorable, that is, more stable. The general principle of molecule formation is illustrated in Figure 1.3a, showing two atoms brought together from infinity. As the two atoms approach each other, the atoms exert attractive and repulsive forces on each other as a result of mutual electrostatic interactions. Initially, the attractive force  $F_A$  dominates over the repulsive force  $F_R$ . The net force  $F_N$  is the sum of the two,

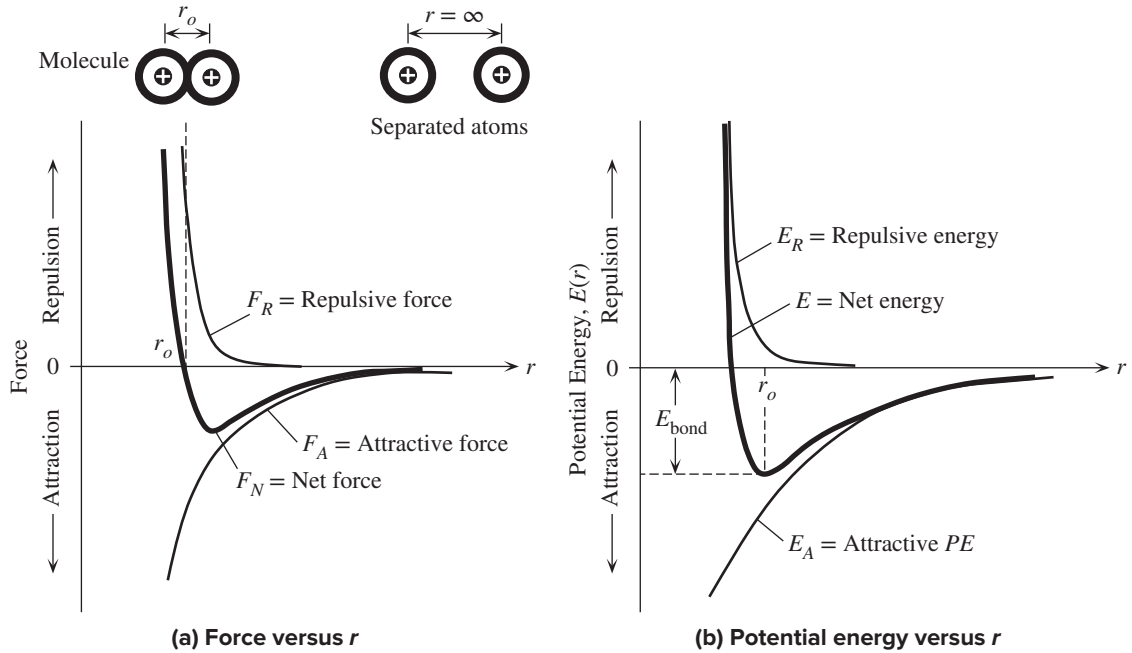
$$F_N = F_A + F_R$$

*Net force*

and this is initially attractive, as indicated in Figure 1.3a. Note that we have defined the attractive force as negative and repulsive force as positive in Figure 1.3a.<sup>5</sup>

<sup>5</sup> In some materials science books and in the third edition of this book, the attractive force is shown as positive, which is an arbitrary choice. A positive attractive force is more appealing to our intuition.





**Figure 1.3** (a) Force versus interatomic separation and (b) potential energy versus interatomic separation. Note that the negative sign represents attraction.

The potential energy  $E(r)$  of the two atoms can be found from<sup>6</sup>

Net force and potential energy

$$F_N = -\frac{dE}{dr}$$

by integrating the net force  $F_N$ . Figure 1.3a and b show the variation of the net force  $F_N(r)$  and the overall potential energy  $E(r)$  with the interatomic separation  $r$  as the two atoms are brought together from infinity. The lowering of energy corresponds to an attractive interaction between the two atoms.

The variations of  $F_A$  and  $F_R$  with distance are different. Force  $F_A$  varies slowly, whereas  $F_R$  varies strongly with separation and is strongest when the two atoms are very close. When the atoms are so close that the individual electron shells overlap, there is a very strong electron-to-electron shell repulsion and  $F_R$  dominates. An equilibrium will be reached when the attractive force just balances the repulsive force and the net force is zero, or

Net force in bonding between atoms

$$F_N = F_A + F_R = 0 \quad [1.3]$$

In this state of equilibrium, the atoms are separated by a certain distance  $r_o$ , as shown in Figure 1.3. This distance is called the **equilibrium separation** and is effectively

<sup>6</sup> Remember that the change  $dE$  in the PE is the work done by the force,  $dE = -F_N dr$ . In Figure 1.3b, when the atoms are far separated,  $dE/dr$  is negative, which represents an attractive force.