2.1 INTRODUCTION

Some of the important properties of solid materials depend on geometrical atomic arrangements, and also the interactions that exist among constituent atoms or molecules. This chapter, by way of preparation for subsequent discussions, considers several fundamental and important concepts—namely, atomic structure, electron configurations in atoms and the periodic table, and the various types of primary and secondary interatomic bonds that hold together the atoms comprising a solid. These topics are reviewed briefly, under the assumption that some of the material is familiar to the reader.

Atomic Structure

2.2 FUNDAMENTAL CONCEPTS

Each atom consists of a very small nucleus composed of protons and neutrons, which is encircled by moving electrons. Both electrons and protons are electrically charged, the charge magnitude being 1.60×10^{-19} C, which is negative in sign for electrons and positive for protons; neutrons are electrically neutral. Masses for these subatomic particles are infinitesimally small; protons and neutrons have approximately the same mass, 1.67×10^{-27} kg, which is significantly larger than that of an electron, 9.11×10^{-31} kg.

atomic number

Each chemical element is characterized by the number of protons in the nucleus, or the **atomic number** (Z).[1] For an electrically neutral or complete atom, the atomic number also equals the number of electrons. This atomic number ranges in integral units from 1 for hydrogen to 92 for uranium, the highest of the naturally occurring elements.

The *atomic mass* (A) of a specific atom may be expressed as the sum of the masses of protons and neutrons within the nucleus. Although the number of protons is the same for all atoms of a given element, the number of neutrons (N) may be

isotope

variable. Thus atoms of some elements have two or more different atomic masses, which are called **isotopes.** The **atomic weight** of an element corresponds to the

atomic weight

weighted average of the atomic masses of the atom's naturally occurring isotopes.[2]

atomic mass unit

The **atomic mass unit (amu)** may be used for computations of atomic weight. A

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[1] Terms appearing in boldface type are defined in the Glossary, which follows Appendix E.
[2] The term "atomic mass" is really more accurate than "atomic weight" inasmuch as, in this context, we are dealing with masses and not weights. However, atomic weight is, by convention, the preferred terminology and will be used throughout this book. The reader should note that it is *not* necessary to divide molecular weight by the gravitational constant.

scale has been established whereby 1 amu is defined as $\frac{1}{12}$ of the atomic mass of the most common isotope of carbon, carbon 12 (^{12}C) ($A = 12.00000$). Within this scheme, the masses of protons and neutrons are slightly greater than unity, and

$$A \cong Z + N \tag{2.1}$$

The atomic weight of an element or the molecular weight of a compound may be specified on the basis of amu per atom (molecule) or mass per mole of material. In one **mole** of a substance there are 6.023×10^{23} (Avogadro's number) atoms or molecules. These two atomic weight schemes are related through the following equation:

$$1 \text{ amu/atom (or molecule)} = 1 \text{ g/mol}$$

For example, the atomic weight of iron is 55.85 amu/atom, or 55.85 g/mol. Sometimes use of amu per atom or molecule is convenient; on other occasions g (or kg)/mol is preferred. The latter is used in this book.

mole

✓ *Concept Check 2.1*

Why are the atomic weights of the elements generally not integers? Cite two reasons.

[*The answer may be found at www.wiley.com/college/callister (Student Companion Site).*]
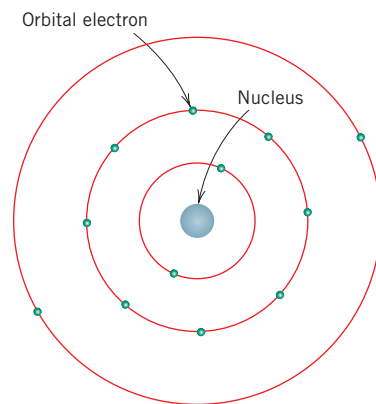
2.3 ELECTRONS IN ATOMS

Atomic Models

During the latter part of the nineteenth century it was realized that many phenomena involving electrons in solids could not be explained in terms of classical mechanics. What followed was the establishment of a set of principles and laws that govern systems of atomic and subatomic entities that came to be known as **quantum mechanics.** An understanding of the behavior of electrons in atoms and crystalline solids necessarily involves the discussion of quantum-mechanical concepts. However, a detailed exploration of these principles is beyond the scope of this book, and only a very superficial and simplified treatment is given.

quantum mechanics

One early outgrowth of quantum mechanics was the simplified **Bohr atomic model,** in which electrons are assumed to revolve around the atomic nucleus in discrete orbitals, and the position of any particular electron is more or less well defined in terms of its orbital. This model of the atom is represented in Figure 2.1.

Bohr atomic model

Another important quantum-mechanical principle stipulates that the energies of electrons are quantized; that is, electrons are permitted to have only specific values of energy. An electron may change energy, but in doing so it must make a quantum jump either to an allowed higher energy (with absorption of energy) or to a lower energy (with emission of energy). Often, it is convenient to think of these allowed electron energies as being associated with *energy levels* or *states*. These states do not vary continuously with energy; that is, adjacent states are separated by finite energies. For example, allowed states for the Bohr hydrogen atom are represented in Figure 2.2*a*. These energies are taken to be negative, whereas the zero reference is the unbound or free electron. Of course, the single electron associated with the hydrogen atom will fill only one of these states.

**18   •   Chapter 2   /   Atomic Structure and Interatomic Bonding**

Figure 2.1   Schematic representation of the Bohr atom.

Thus, the Bohr model represents an early attempt to describe electrons in atoms, in terms of both position (electron orbitals) and energy (quantized energy levels).

This Bohr model was eventually found to have some significant limitations because of its inability to explain several phenomena involving electrons. A resolution was reached with a **wave-mechanical model,** in which the electron is considered to exhibit both wave-like and particle-like characteristics. With this model, an electron is no longer treated as a particle moving in a discrete orbital; rather, position is considered to be the probability of an electron's being at various locations around the nucleus. In other words, position is described by a probability distribution or electron cloud. Figure 2.3 compares Bohr and wave-mechanical models for the hydrogen atom. Both these models are used throughout the course of this book; the choice depends on which model allows the more simple explanation.

wave-mechanical model
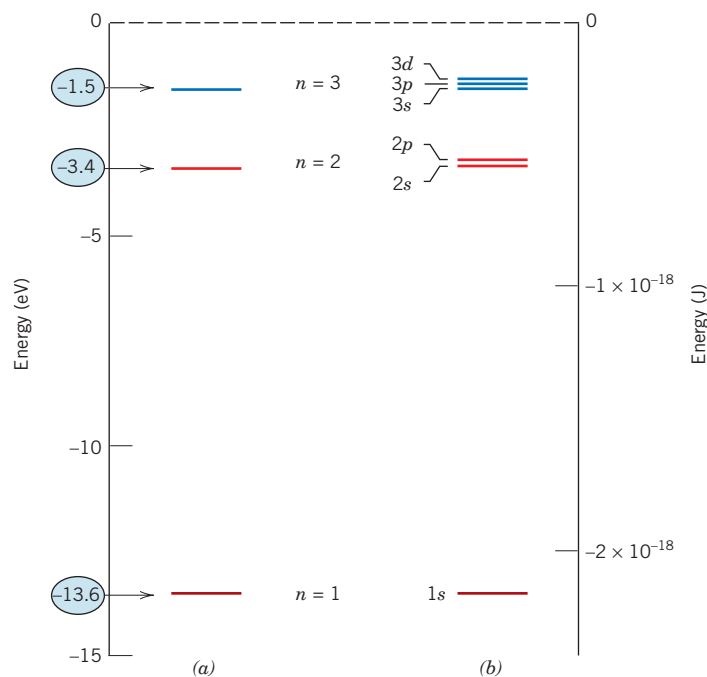
Figure 2.2   (*a*) The first three electron energy states for the Bohr hydrogen atom. (*b*) Electron energy states for the first three shells of the wave-mechanical hydrogen atom. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials,* Vol. I, *Structure,* p. 10. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)