Chapter 2

Chapter 2: Atomic Structure and Interatomic Bonding

2.1 Introduction

- **Key Idea**: Understanding atomic structure and bonding is essential for explaining the properties of materials.
- **Focus**: How atomic arrangements and bonding types influence material properties.

2.2 Fundamental Concepts

- **Atomic Structure**: Atoms consist of protons, neutrons, and electrons.
- **Definitions**:
  - **Atomic Number (Z)**: Number of protons in an atom's nucleus.
  - **Atomic Mass (A)**: Sum of protons and neutrons.
  - **Atomic Weight**: Weighted average of the atomic masses of an element's isotopes.
  - **Isotopes**: Atoms with the same number of protons but different numbers of neutrons.

  Example Problem: Calculating the average atomic weight for isotopes of cerium.

2.3 Electrons in Atoms

- **Quantum Mechanics**: Electrons behave according to quantum mechanical principles.
  - **Bohr Model**: Electrons move in discrete orbits around the nucleus.
  - **Wave-Mechanical Model**: Electrons have wavelike properties, and their position is described by probability distributions.
  - **Electron Configuration**: Arrangement of electrons in an atom's orbitals, governed by four quantum numbers:
    - **n**: Principal quantum number (size of the orbital).
    - **l**: Angular momentum quantum number (shape of the orbital).
    - **m_l**: Magnetic quantum number (orientation of the orbital).
    - **m_s**: Spin quantum number (electron spin direction).
  - **Pauli Exclusion Principle**: No two electrons can have the same set of four quantum numbers.

2.4 The Periodic Table

- **Arrangement**: Elements are arranged based on their atomic number, and their properties vary systematically across periods and groups.
- **Electronegativity**: Tendency of an atom to attract electrons.
  - Electronegativity increases from left to right and from bottom to top in the periodic table.

  Figure: The periodic table highlighting electronegativity trends.

2.5 Bonding Forces and Energies

- **Key Concept**: The stability and properties of materials depend on the forces between atoms.
- **Bonding Forces**:
  - **Attractive Forces (F_A)**: Depend on the type of bonding between atoms.
  - **Repulsive Forces (F_R)**: Arise due to the overlap of electron clouds at short distances.
- **Bonding Energy (E_0)**: Minimum energy required to separate two bonded atoms; relates directly to melting temperature and stiffness of materials. **Figure 2.10**: Plot of attractive, repulsive, and net energies vs. interatomic separation.

2.6 Primary Interatomic Bonds

- **Ionic Bonding**:
  - Occurs between metals and nonmetals, involves electron transfer.
  - Example: NaCl, where Na donates an electron to Cl.
  - **Properties**: High bonding energies, typically found in ceramics.

  Figure 2.11: Formation of Na^+ and Cl^- ions and the resulting ionic bond.
- **Covalent Bonding**:
  - Involves electron sharing between atoms with similar electronegativities.
  - **Example**: Hydrogen molecule (H_2) and diamond (C).
  - **Properties**: Covalent bonds can be very strong, leading to materials like diamond.

  Figure 2.12: Covalent bonding between two hydrogen atoms.
- **Metallic Bonding**:
  - Involves a "sea of electrons" that is shared among all metal atoms.
  - **Properties**: Metals are good conductors of electricity and are ductile due to this bonding mechanism.

  Figure 2.19: Schematic illustration of metallic bonding.

2.7 Secondary Bonding or van der Waals Bonding

- **Secondary Bonds**:
  - **Van der Waals Bonds**: Weak forces between atoms or molecules due to induced dipoles.
  - **Hydrogen Bonding**: A special type of dipole-dipole interaction involving hydrogen.

- **Properties**: Lower bonding energies, found in molecular solids (e.g., water).

Figure 2.20: Dipole interactions in van der Waals bonding.

2.8 Mixed Bonding

- **Mixed Bonds**: Many materials exhibit a combination of bonding types, such as ionic-covalent or covalent-metallic.
- **Percent Ionic Character (%IC)**: Indicates the degree to which a bond between two atoms is ionic. **Equation 2.16**: Calculation of %IC based on electronegativities.

2.9 Molecules

- **Molecular Solids**: Solids composed of molecules held together by van der Waals forces.
- **Example**: Polymers, which often exhibit covalent bonds within molecules and van der Waals bonds between molecules.

2.10 Bonding Type-Material Classification Correlations

- **Correlations**: The type of bonding influences the material classification:
  - **Polymers**: Covalent bonding within molecules.
  - **Metals**: Metallic bonding.
  - **Ceramics**: Ionic and/or covalent bonding.
  - **Molecular Solids**: Van der Waals bonding.

Figure 2.25: Bonding tetrahedron showing correlations between material types and bonding.

Important Definitions:

- **Ionic Bonding**: Transfer of electrons from one atom to another.
- **Covalent Bonding**: Sharing of electrons between atoms.
- **Metallic Bonding**: Electrons shared in a "sea" among many atoms.
- **van der Waals Bonding**: Weak intermolecular forces due to temporary dipoles.
- **Bonding Energy (E_o)**: Energy required to break a bond.
- **Electronegativity**: Ability of an atom to attract electrons.