General Characteristics of Materials: First Principles

Nate

September 5, 2025

Contents

1 Introduction

First week of the course focuses on the fundamental characteristics of materials, including their mechanical properties and how they respond to various forces.

2 Materials

2.1 Ceramics

Salts – ionic bonding, brittle, high melting points, poor conductors of electricity and heat. Ex. alumina (Al_2O_3), silicon carbide (SiC), and zirconia (ZrO_2).
spacing

ceramics

2.2 Metals

Metalic bonding is strong. Metals are ductile, malleable, and good conductors of electricity and heat. They typically have high melting points and are often used in structural applications. Ex. aluminum, copper, iron, and steel.
spacing

metals Metalic Bonding

metals Variable Bond Energy

metals moderate T_m

metals moderate E

metals moderate α

2.3 Polymers

Polymers are made up of long chains of repeating molecular units. They can be flexible or rigid, and their properties can vary widely depending on their chemical structure and the way they are processed. Polymers are generally poor conductors of heat and electricity, and they can be engineered to have specific mechanical properties such as toughness or elasticity. Ex. polyethylene, polystyrene, and nylon.

Polymers have a small melting point because they have weak bonds.
spacing

Polymers Covalent and Secondary Bonds

Polymers Secondary bonding dominates

Polymers Directional properties

Polymers small T_m

Polymers small E

Polymers large α

2.4 Composites

Composites are materials made from two or more constituent materials with significantly different physical or chemical properties. When combined, they produce a material with characteristics different from the individual components. Ex. wood (cellulose fibers in a lignin matrix), fiberglass (glass fibers in a polymer matrix).

3 Bonding Types

3.1 Primary Bonds

Primary bonding: ionic - transfer of electrons, covalent - sharing of electrons, metallic bond - delocalized cloud of electrons,

$$\%\text{ Ionic Character } = (1 - e^{-\frac{(\chi_A - \chi_B)^2}{4}}) \times 100\%$$

where χ_A and χ_B are the electronegativities of atoms A and B, respectively.

3.2 Secondary Bonds

Van der Walls forces, dipole-dipole interactions, hydrogen bonding are caused by the attraction/repulsion of charged particles or dipoles in molecules. These forces are generally weaker than primary bonds but can significantly influence the physical properties of materials, such as melting point and solubility.

4 Energy of the Bonds

Energy = Force * Distance.

$$E_N = E_A + E_R = -\frac{A}{r} + \frac{B}{r^n}$$

n is the Leanord Jones Potential and is generally 8 or 9. r is the distance between atoms. E_N is the Net Energy. r_0 is the equilibrium distance between the two atoms.

To find r_0, find the E_N equation derivative and set it equal to 0. Then, plug r_0 back in to the original equation to get E_0.

IMPORTANT SUMMARY T_m is larger if E_0 is larger. α is larger if E0 is smaller / well-size. α is the coefficient of thermal expansion. E is larger whichever is steepest.

Ex. Test Question: *Van der Waals bonds most commonly occur in polymers and result in low melting temperatures.*

5 Equations

Stress: $\sigma = \frac{F}{A}$