INTERATOMIC POTENTIALS

- Bond length, \( r \)
- Bond energy, \( E_0 \)
- Melting Temperature, \( T_m \)

\( E_0 = \) "bond energy"

\( T_m \) is larger if \( E_0 \) is larger.
PROPERTIES FROM BONDING: \( E \)

- Elastic modulus, \( E \)
  \[ \frac{F}{A_0} = E \frac{\Delta L}{L_0} \]

  - \( E \sim \) curvature at \( r_0 \)

  - \( E \) is larger if \( E_0 \) is larger.

- Energy

PROPERTIES FROM BONDING: \( \alpha \)

- Coefficient of thermal expansion, \( \alpha \)
  \[ \frac{\Delta L}{L_0} = \alpha (T_2 - T_1) \]

  - \( \alpha \sim \) symmetry at \( r_0 \)

  - \( \alpha \) is larger if \( E_0 \) is smaller.
### SUMMARY: PRIMARY BONDS

<table>
<thead>
<tr>
<th>Material</th>
<th>Bond Energy</th>
<th>Melting Temperature</th>
<th>Elasticity</th>
<th>Directional Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ceramics</td>
<td>Large bond energy</td>
<td>large $T_m$</td>
<td>large $E$</td>
<td>small $\alpha$</td>
</tr>
<tr>
<td>Ionic &amp; covalent bonding</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Metals</td>
<td>Variable bond energy</td>
<td>moderate $T_m$</td>
<td>moderate $E$</td>
<td>moderate $\alpha$</td>
</tr>
<tr>
<td>Metallic bonding</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Polymers</td>
<td>Directional Properties</td>
<td>Small $T$</td>
<td>small $E$</td>
<td>large $\alpha$</td>
</tr>
<tr>
<td>(Covalent &amp; Secondary)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### CHAPTER 3: CRYSTAL STRUCTURES & PROPERTIES

### ISSUES TO ADDRESS...

- How do atoms assemble into solid structures? (for now, focus on metals)
- How does the density of a material depend on its structure?
- When do material properties vary with the sample (i.e., part) orientation?
ENERGY AND PACKING

- Non dense, random packing
  - Dense, regular packing

Dense, regular-packed structures tend to have lower energy.

CRYSTALLINE MATERIALS

AFM image of Au surface

TEM Image of $\text{Sc}_2\text{O}_3$
(S. Stemmer)
MATERIALS AND PACKING

Crystalline materials...
• atoms pack in periodic, 3D arrays
• typical of: -metals
  -many ceramics
  -some polymers

Noncrystalline materials...
• atoms have no periodic packing
• occurs for: -complex structures
  -rapid cooling

"Amorphous" = Noncrystalline

METALLIC CRYSTALS

• Tend to be densely packed.
• Several reasons for dense packing:
  -Typically, only one element is present, so all atomic radii are the same.
  -Metallic bonding has weak directionallity.
  -Nearest neighbor distances tend to be small to lower bond energy.

• Metals have the simplest crystal structures.
  We will look at three such structures...
SIMPLE CUBIC STRUCTURE (SC)

- Rare due to poor packing (only Po has this structure)
  \( \text{Po} = \text{Polonium! } Z = 84 \)
- Close-packed directions are cube edges.
  - Coordination \# = 6
    \(#\) nearest neighbors

ATOMIC PACKING FACTOR

\[ \text{APF} = \frac{\text{Volume of atoms in unit cell} \ast}{\text{Volume of unit cell}} \]
*assume hard spheres

- APF for a simple cubic structure = 0.52

\[ \text{APF} = \frac{1}{3} \pi (0.5a)^3 \]

Adapted from Fig. 3.19, Callister 6e.
BODY CENTERED CUBIC STRUCTURE (BCC)

• Close packed directions are cube diagonals
• Coordination # = 8

ATOMIC PACKING FACTOR: BCC

• APF for a body-centered cubic structure = 0.68

Close-packed directions:
length = 4R
= $\sqrt{3} a$

Unit cell contains:
1 + 8 x $1/8$
= 2 atoms/unit cell

Adapted from Fig. 3.2, Callister 6e.
FACE CENTERED CUBIC STRUCTURE (FCC)

- Close packed directions are face diagonals
- Coordination # = 12

![Diagram of FCC structure](image)

**ATOMIC PACKING FACTOR: FCC**

- APF for a body-centered cubic structure = 0.74

Close-packed directions:
- length = 4R
  \[= \sqrt{2} \ a\]

Unit cell contains:
- \(6 \times \frac{1}{2} + 8 \times \frac{1}{8}\)
- = 4 atoms/unit cell

![Diagram showing atomic packing factor](image)
FCC STACKING SEQUENCE

• ABCABC... Stacking Sequence
• 2D Projection

A sites
B sites
C sites

• FCC Unit Cell

HEXAGONAL CLOSE-PACKED STRUCTURE (HCP)

• ABAB... Stacking Sequence
• 3D Projection

A sites
B sites
A sites

• Coordination # = 12
• APF = 0.74

• 2D Projection

Top layer
Middle layer
Bottom layer

Adapted from Fig. 3.3, Callister 6e.
STRUCTURE OF COMPOUNDS: NaCl

- Compounds: Often have similar close-packed structures.
- Structure of NaCl
- Close-packed directions --along cube edges.

Example: Copper

Data from Table inside front cover of Callister (see next slide):
- crystal structure = FCC: 4 atoms/unit cell
- atomic weight = 63.55 g/mol (1 amu = 1 g/mol)
- atomic radius R = 0.128 nm (1 nm = 10^{-7} cm)
  \[ V_c = a^3 \; \text{For FCC,} \; a = 4R/\sqrt{3}; \; V_c = 4.75 \times 10^{-23} \text{cm}^3 \]

Result: theoretical \( \rho_{\text{Cu}} = 8.89 \text{ g/cm}^3 \)
Compare to actual: \( \rho_{\text{Cu}} = 8.94 \text{ g/cm}^3 \)

THEORETICAL DENSITY, \( \rho \)

\[ \rho = \frac{n A}{V_c N_A} \]

- # atoms/unit cell
- Volume/unit cell (cm^3/unit cell)
- Atomic weight (g/mol)
- Avogadro's number (6.023 \times 10^{23} \text{ atoms/mol})
### Characteristics of Selected Elements at 20 °C

<table>
<thead>
<tr>
<th>Element</th>
<th>Symbol</th>
<th>At. Weight (amu)</th>
<th>Density (g/cm³)</th>
<th>Crystal Structure</th>
<th>Atomic radius (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>Al</td>
<td>26.98</td>
<td>2.71</td>
<td>FCC</td>
<td>0.143</td>
</tr>
<tr>
<td>Argon</td>
<td>Ar</td>
<td>39.95</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>Barium</td>
<td>Ba</td>
<td>137.33</td>
<td>3.5</td>
<td>BCC</td>
<td>0.217</td>
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<tr>
<td>Beryllium</td>
<td>Be</td>
<td>9.012</td>
<td>1.85</td>
<td>HCP</td>
<td>0.114</td>
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<tr>
<td>Boron</td>
<td>B</td>
<td>10.81</td>
<td>2.34</td>
<td>Rhomb</td>
<td>-----</td>
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<tr>
<td>Bromine</td>
<td>Br</td>
<td>79.90</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
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<tr>
<td>Cadmium</td>
<td>Cd</td>
<td>112.41</td>
<td>8.65</td>
<td>HCP</td>
<td>0.149</td>
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<tr>
<td>Calcium</td>
<td>Ca</td>
<td>40.08</td>
<td>1.55</td>
<td>FCC</td>
<td>0.197</td>
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<tr>
<td>Carbon</td>
<td>C</td>
<td>12.011</td>
<td>2.25</td>
<td>Hex</td>
<td>0.071</td>
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<tr>
<td>Cesium</td>
<td>Cs</td>
<td>132.91</td>
<td>1.87</td>
<td>BCC</td>
<td>0.265</td>
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<tr>
<td>Chlorine</td>
<td>Cl</td>
<td>35.45</td>
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<tr>
<td>Chromium</td>
<td>Cr</td>
<td>52.00</td>
<td>7.19</td>
<td>BCC</td>
<td>0.125</td>
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<tr>
<td>Cobalt</td>
<td>Co</td>
<td>58.93</td>
<td>8.9</td>
<td>HCP</td>
<td>0.125</td>
</tr>
<tr>
<td>Copper</td>
<td>Cu</td>
<td>63.55</td>
<td>8.94</td>
<td>FCC</td>
<td>0.128</td>
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<tr>
<td>Flourine</td>
<td>F</td>
<td>19.00</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
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<tr>
<td>Gallium</td>
<td>Ga</td>
<td>69.72</td>
<td>5.90</td>
<td>Ortho.</td>
<td>0.122</td>
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<tr>
<td>Germanium</td>
<td>Ge</td>
<td>72.59</td>
<td>5.32</td>
<td>Dia. cubic</td>
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<tr>
<td>Gold</td>
<td>Au</td>
<td>196.97</td>
<td>19.32</td>
<td>FCC</td>
<td>0.144</td>
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<tr>
<td>Helium</td>
<td>He</td>
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<tr>
<td>Hydrogen</td>
<td>H</td>
<td>1.008</td>
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</tbody>
</table>

Adapted from Table, "Characteristics of Selected Elements", inside front cover, Callister 6e.

### DENSITIES OF MATERIAL CLASSES

<table>
<thead>
<tr>
<th>ρ (g/cm³)</th>
<th>Metals</th>
<th>Ceramics</th>
<th>Polymers</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 0.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.3 - 0.5</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>0.5 - 1.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.0 - 2.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.0 - 3.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.0 - 4.0</td>
<td></td>
<td></td>
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<td>4.0 - 5.0</td>
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<td>5.0 - 6.0</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>6.0 - 7.0</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>7.0 - 8.0</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>8.0 - 9.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9.0 - 10.0</td>
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<td></td>
</tr>
<tr>
<td>≥ 10.0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Why?**

**Metals** have...
- close-packing (metallic bonding)
- large atomic mass

**Ceramics** have...
- less dense packing (covalent bonding)
- often lighter elements

**Polymers** have...
- poor packing (often amorphous)
- lighter elements (C,H,O)

**Composites** have...
- intermediate values

---

Based on data in Table B1, Callister 6e.

"GFRE, CFRE, & AFRE are Glass, Carbon, & Aramid Fiber-Reinforced Epoxy composites (values based on 60% volume fraction of aligned fibers in an epoxy matrix)."

Data from Table B1, Callister 6e.
CRYSTALLOGRAPHY I: UNIT CELL

Unit cell: Basic repeat unit

a, b, c: cell dimensions
α, β, γ: interaxial angles

a, b, c: translation vectors

CRYSTALLOGRAPHY II: COORDINATES

Point P:
Coordinates: q r s
qa: along x-axis
rb: along y-axis
sc: along z-axis
CRYSTALLOGRAPHY III: DIRECTIONS

Direction $[u \ v \ w] = ua + vb + wc$

$a, b, c$: translation vectors

Example: $[1 \ 1 \ 0]$

<>

Examples

Specific directions: $[u \ v \ w]$

$[100], [110], [111]$ directions

Families of directions: $<u \ v \ w >$

$\langle 100 \rangle: [100], [001], [00\bar{1}], [10\bar{1}], [\bar{1}0\bar{1}], [\bar{1}01]$