Introduction to Engineering Materials
ENGR2000
Chapter 3: The Structure of Crystalline Solids

Dr. Coates
Learning Objectives I

1. Describe difference in atomic/molecular structure between crystalline/noncrystalline
2. Draw unit cells for FCC, BCC, HCP
3. Derive the relationship between unit cell edge length and atomic radius for FCC, BCC
4. Compute the densities for metals having FCC, BCC given unit cell dimensions
5. Sketch crystallographic directions within unit cells
The **structure** of a material
- arrangement of its internal components

- **Subatomic structure**
  - Electrons & nuclei within the individual atoms

- **Atomic structure**
  - Atoms & molecules within the material

- **Microscopic structure**
  - Large groups of atoms aggregated together

- **Macroscopic structure**
  - Elements that may be viewed with the naked eye
3.2 Fundamental Concepts

- **Crystalline materials**
  - Atoms are situated in a repeating or periodic array over large atomic distances
  - Long-range order

- **Non-crystalline materials (amorphous materials)**
  - Do not have long-range order
  - May have short-range order
3.2 Fundamental Concepts

• Atomic hard sphere model
  – Atoms or ions are thought of as being solid spheres having well-defined diameters.
  – Spheres representing nearest-neighbor atoms touch one another.
3.2 Fundamental Concepts

- Lattice
  - A 3-D array of points coinciding with atomic positions
3.3 Unit Cells

- In describing crystal structures, it is often convenient to subdivide the structure into small repeat entities called unit cells.
3.4 Metallic Crystal Structures

- Atomic bonding is metallic
  Directional or non-directional?
  Would number of nearest neighbor atoms be large or small then?

How about density of atomic packing? Large or small?
3.4 Metallic Crystal Structures

- Crystal structures of common metals
  - Face-centered cubic crystal structure
  - Body-centered cubic crystal structures
  - Hexagonal close-packed crystal structure
Face-Centered Cubic (FCC) Crystal Structure

**Figure 3.1**  For the face-centered cubic crystal structure: (a) a hard sphere unit cell representation, (b) a reduced-sphere unit cell, and (c) an aggregate of many atoms. (Figure c adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)
Face-Centered Cubic (FCC) Crystal Structure

Class exercise: Determine the relationship between $a$ and $R$ for an FCC?

The lattice parameter:

\[ a\sqrt{2} = 4R \]

\[ \Rightarrow a(FCC) = 2R\sqrt{2} \]
Face-Centered Cubic (FCC) Crystal Structure

- The total number of atoms per unit cell
  - How many corner atoms? 8
  - each corner atom is shared by ? cells 8
  - How many face atoms? 6
  - each face atom is shared by ? unit cells 2

\[ total\ number\ of\ atoms\ per\ unit\ cell = \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4 \]
Face-Centered Cubic (FCC) Crystal Structure

- The coordination number (CN)
  - Number of nearest-neighbor
  - or touching atoms

\[ CN(FCC) = 12 \]
Face-Centered Cubic (FCC) Crystal Structure

Atomic Packing Factor (APF):

\[
APF = \frac{\text{volume of atoms in the unit cell}}{\text{total volume of the unit cell}} \quad \text{or} \quad APF = \frac{(\text{number of atoms in the unit cell}) \times (\text{volume of an atom})}{\text{total volume of the unit cell}}
\]
Example 3.1

- Calculate the volume of an FCC unit cell in terms of the atomic radius $R$.

The lattice parameter:

\[ a(FCC) = 2R\sqrt{2} \]

Volume of unit cell:

\[ V = a^3 = (2R\sqrt{2})^3 = 16R^3 \sqrt{2} \]
Example 3.2

- Show that the APF for the FCC structure is 0.74.

\[
APF = \frac{\text{number of atoms in cell} \times \text{volume of an atom}}{\text{total volume of the unit cell}}
\]

\[
= \frac{4 \times \frac{4}{3} \pi R^3}{a^3} = \frac{4 \times \frac{4}{3} \pi R^3}{(2R\sqrt{2})^3} = 0.74
\]
Face-Centered Cubic (FCC) Crystal Structure

- CN of 12
  - Maximum possible for spheres with same diameter.
- APF of 0.74
  - Maximum possible for spheres with same diameter.
### Table 3.1 Atomic Radii and Crystal Structures for 16 Metals

<table>
<thead>
<tr>
<th>Metal</th>
<th>Crystal Structure&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Atomic Radius&lt;sup&gt;b&lt;/sup&gt; (nm)</th>
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<tbody>
<tr>
<td>Aluminum</td>
<td>FCC</td>
<td>0.1431</td>
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<td>0.1363</td>
</tr>
<tr>
<td>Cadmium</td>
<td>HCP</td>
<td>0.1490</td>
<td>Nickel</td>
<td>FCC</td>
<td>0.1246</td>
</tr>
<tr>
<td>Chromium</td>
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</tr>
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<td>Cobalt</td>
<td>HCP</td>
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<td>FCC</td>
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<tr>
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<sup>a</sup> FCC = face-centered cubic; HCP = hexagonal close-packed; BCC = body-centered cubic.

<sup>b</sup> A nanometer (nm) equals $10^{-9}$ m; to convert from nanometers to angstrom units (Å), multiply the nanometer value by 10.
Body-Centered Cubic (BCC) Crystal Structure

**Figure 3.2** For the body-centered cubic crystal structure, (a) a hard sphere unit cell representation, (b) a reduced-sphere unit cell, and (c) an aggregate of many atoms. (Figure c from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)
Body-Centered Cubic (BCC) Crystal Structure

The lattice parameter:

\[ \frac{a \sqrt{3}}{2} = 2R \]

\[ \Rightarrow a(BCC) = \frac{4R}{\sqrt{3}} \]
Body-Centered Cubic (BCC) Crystal Structure

- The total number of atoms per unit cell
  - each corner atom is shared by 8 cells
  - hence, only 1/8 of each corner atom is contained within each cell
  - the center atom is totally contained within the cell

\[ \text{total number of atoms per unit cell} = (1/8 \times 8) + (1 \times 1) = 2 \]
Body-Centered Cubic (BCC) Crystal Structure

- The coordination number
  - Number of nearest-neighbor or touching atoms

\[ CN(BCC) = 8 \]
Body-Centered Cubic (BCC) Crystal Structure

• CN of 8
  – Less than that of the FCC structure.

• APF of 0.68
  – Less than that of the FCC structure.
Table 3.1  Atomic Radii and Crystal Structures for 16 Metals

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<sup>b</sup> A nanometer (nm) equals $10^{-9}$ m; to convert from nanometers to angstrom units (Å), multiply the nanometer value by 10.
Hexagonal Close-Packed (HCP) Crystal Structure

**Figure 3.3** For the hexagonal close-packed crystal structure, (a) a reduced-sphere unit cell ($a$ and $c$ represent the short and long edge lengths, respectively), and (b) an aggregate of many atoms. (Figure b from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, Structure, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)
Hexagonal Close-Packed (HCP) Crystal Structure

- The total number of atoms per cell
  - six atoms at the corners of the top and bottom planes (basal planes)
  - shared by six unit cells
  - one atom in the center of the top and bottom planes (shared by two unit cells)
  - three atoms in the midplane

Total number of atoms per cell of HCP = \( \frac{1}{6} \times 12 \) + \( \frac{1}{2} \times 2 \) + \( 1 \times 3 \) = 6
Hexagonal Close-Packed (HCP) Crystal Structure

The short & long unit cell dimensions:

\[
\frac{c}{a} = \frac{4}{\sqrt{6}} = 1.633
\]

- for the ideal HCP unit cell
- assuming the atoms are perfect rigid spheres
Hexagonal Close-Packed (HCP) Crystal Structure

- The coordination number
  - Number of nearest-neighbor or touching atoms

\[ CN(HCP) = 12 \]
Hexagonal Close-Packed (HCP) Crystal Structure

- CN of 12
  - Maximum possible for spheres with same diameter.
- APF of 0.74
  - Maximum possible for spheres with same diameter.
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3.5 Density Computations

- A knowledge of the crystal structure of a metallic solid permits computation of its theoretical density:

\[ \rho = \frac{nA}{V_C N_A} \]

where \( n \) is the number of atoms in each unit cell,
\( A \) is the atomic weight,
\( V_C \) is the volume of the unit cell and
\( N_A \) is the Avogadro's number.
Example 3.4

- Copper has an atomic radius of 0.128 nm, an FCC crystal structure and an atomic weight of 63.5 g/mol. Compute its theoretical density and compare with its measured density.
Example 3.4

Given:
- Cu has an FCC structure

\[ A = 63.5 \text{ g/mol} \]
\[ r = 0.128 \text{ nm} \]

Theoretical density:

\[ \rho = \frac{nA}{V_C N_A} \]

\[ = \frac{4 \times 63.5 \text{ g/mol}}{\left(16 \left(0.128 \times 10^{-7} \text{ cm}\right)^3 \sqrt{2}\right) \left(6.023 \times 10^{23}\right)} \]

\[ = 8.89 \text{ g/cm}^3 \]

Measured density = 8.94 g/cm³
3.6 Polymorphism and Allotropy

- Polymorphism
  - Some metals/non-metals have more than one crystal structure

- Allotropy
  - Elemental solids with more than one crystal structure
  - Carbon as graphite or diamond
3.7 Crystal Systems

There are seven crystal systems based on unit cell geometry.

**Figure 3.4** A unit cell with $x$, $y$, and $z$ coordinate axes, showing axial lengths ($a$, $b$, and $c$) and interaxial angles ($\alpha$, $\beta$, and $\gamma$).

**Lattice parameters:**

$a, b, c$

$\alpha, \beta, \gamma$

There are seven crystal systems based on unit cell geometry.
<table>
<thead>
<tr>
<th>Crystal System</th>
<th>Axial Relationships</th>
<th>Interaxial Angles</th>
<th>Unit Cell Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic</td>
<td>$a = b = c$</td>
<td>$\alpha = \beta = \gamma = 90^\circ$</td>
<td></td>
</tr>
<tr>
<td>Hexagonal</td>
<td>$a = b \neq c$</td>
<td>$\alpha = \beta = 90^\circ, \gamma = 120^\circ$</td>
<td></td>
</tr>
<tr>
<td>Tetragonal</td>
<td>$a = b \neq c$</td>
<td>$\alpha = \beta = \gamma = 90^\circ$</td>
<td></td>
</tr>
<tr>
<td>Crystal System</td>
<td>Conditions</td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------------------</td>
<td>----------------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Rhombohedral</td>
<td>$a = b = c$  $\alpha = \beta = \gamma \neq 90^\circ$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>$a \neq b \neq c$  $\alpha = \beta = \gamma = 90^\circ$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Monoclinic</td>
<td>$a \neq b \neq c$  $\alpha = \gamma = 90^\circ \neq \beta$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Triclinic</td>
<td>$a \neq b \neq c$  $\alpha \neq \beta \neq \gamma \neq 90^\circ$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
3.8 Point Coordinates
- Miller Indices

**Figure 3.5** The manner in which the $q$, $r$, and $s$ coordinates at point $P$ within the unit cell are determined. The $q$ coordinate (which is a fraction) corresponds to the distance $qa$ along the $x$ axis, where $a$ is the unit cell edge length. The respective $r$ and $s$ coordinates for the $y$ and $z$ axes are determined similarly.

Coordinates of $P$:

$q, r, s$ fractional multiples of $abc$

Convention:

$q, r, s \leq 1$

- coordinates are not separated by commas
Example 3.5

- Locate the point with coordinates \( \frac{1}{4} 1 \frac{1}{2} \).
Example 3.6

- Specify point coordinates for all atom positions for a BCC unit cell.
3.9 Crystallographic Directions

A vector of convenient length is positioned such that it passes through the origin of the coordinate system. Any vector may be translated throughout the crystal lattice without alteration, if parallelism is maintained.
Crystallographic Directions

Algorithm

1. Determine coordinates of vector tail, pt. 1: \(x_1, y_1, \& \ z_1\); and vector head, pt. 2: \(x_2, y_2, \& \ z_2\).
2. Tail point coordinates subtracted from head point coordinates.
3. Normalize coordinate differences in terms of lattice parameters \(a, b, \& \ c\):
   \[
   \frac{x_2 - x_1}{a} \quad \frac{y_2 - y_1}{b} \quad \frac{z_2 - z_1}{c}
   \]
4. Adjust to smallest integer values
5. Enclose in square brackets, no commas

ex:
pt. 1 \(x_1 = 0, y_1 = 0, z_1 = 0\)
pt. 2 \(x_2 = a, y_2 = 0, z_2 = c/2\)

\[
\begin{align*}
\frac{a - 0}{a} & \quad \frac{0 - 0}{b} & \quad \frac{c/2 - 0}{c} \\
\end{align*}
\]

\(\Rightarrow 1, 0, 1/2\) \(\Rightarrow 2, 0, 1\)

\(\Rightarrow [201]\)
Crystallographic Directions

Example 2:

pt. 1 \( x_1 = a, \ y_1 = b/2, \ z_1 = 0 \)

pt. 2 \( x_2 = -a, \ y_2 = b, \ z_2 = c \)

\[
\frac{-a - a}{a} \quad \frac{b - b/2}{b} \quad \frac{c - 0}{c}
\]

\[=> -2, 1/2, 1\]

Multiplying by 2 to eliminate the fraction

\(-4, 1, 2 \Rightarrow [\bar{4}12]\) where the overbar represents a negative index
3.9 Crystallographic Directions

• For some crystal systems, can have equivalent directions
  – Nonparallel directions with different indices but with same spacing of atoms along each direction
  – Can be grouped into a family of directions \(<uvw>\)

• Cubic crystals
  – \([100],[\overline{1}00],[010],[0\overline{1}0],[001],[00\overline{1}]\) are equivalent
  – Grouped together into the family ex. \(<100>\)
Learning Outcomes met thus far!

1. Describe difference in atomic/molecular structure between crystalline/non-crystalline
2. Draw unit cells for FCC, BCC, HCP
3. Derive the relationship between unit cell edge length and atomic radius for FCC, BCC
4. Compute the densities for metals having FCC, BCC given unit cell dimensions
5. Sketch crystallographic directions within unit cells
HCP Crystallographic Directions

• **Hexagonal Crystals**
  
  – 4 parameter Miller-Bravais lattice coordinates are related to the direction indices (i.e., $uvw$) in the ‘3 space’ Bravais lattice as follows.

$$[U VW ] \rightarrow [uv tw ]$$

$$u = \frac{1}{3}(2U - V)$$

$$v = \frac{1}{3}(2 V - U)$$

$$t = -(u + v)$$

$$w = W$$
Computing HCP Miller- Bravais Directional Indices (an alternative way):

We confine ourselves to the bravais parallelepiped in the hexagon: \( a_1-a_2-Z \) and determine: \((u',v'w')\)

Here: \([1\ 1\ 0]\) - so now apply the models to create M-B Indices

\[
\begin{align*}
    u &= \frac{1}{3} (2u' - v') = \frac{1}{3} (2*1-1) = \frac{1}{3} \rightarrow 1 \\
    v &= \frac{1}{3} (2v' - u') = \frac{1}{3} (2*1-1) = \frac{1}{3} \rightarrow 1 \\
    t &= -(u + v) = -\left( \frac{1}{3} + \frac{1}{3} \right) = -\frac{2}{3} \rightarrow -2 \\
    w &= w' = 0
\end{align*}
\]

M-B Indices: \([11\bar{2}0]\)
Drawing HCP Crystallographic Directions (ii)

• Draw the \([\bar{1} \bar{2} 13]\) direction in a hexagonal unit cell.

Algorithm

1. Remove brackets

\[
\begin{array}{ccc}
a_1 & a_2 & a_3 \\
-1 & -2 & 1 \\
\end{array}
\]

2. Divide by 3

\[
\begin{array}{ccc}
a_1 & a_2 & a_3 \\
\frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\
\end{array}
\]

3. Projections

\[
\begin{array}{ccc}
a_1 & a_2 & a_3 \\
\frac{-a}{3} & \frac{-2a}{3} & \frac{a}{3} \\
\end{array}
\]

4. Construct Vector

- Start at point \(o\)
- Proceed \(-a/3\) units along \(a_1\) axis to point \(p\)
- \(-2a/3\) units parallel to \(a_2\) axis to point \(q\)
- \(a/3\) units parallel to \(a_3\) axis to point \(r\)
- \(c\) units parallel to \(z\) axis to point \(s\)

\([\bar{1} \bar{2} 13]\) direction represented by vector from point \(o\) to point \(s\)
3.10 Crystallographic Planes

1. If the plane passes through the selected origin, another parallel plane must be constructed by translation within the unit cell to another corner.

2. The length of the planar intercept for each axis is determined in terms of the lattice parameters a, b and c.

3. The reciprocals of the above numbers are taken. A plane that parallels an axis is considered to have an infinite intercept.

4. The numbers are changed to the set of smallest integers by multiplication or division by a common factor.

5. The integer indices, not separated by commas, are enclosed within parentheses: 
   \((hkl)\)
3.10 Crystallographic Planes

- Parallel planes are equivalent and have identical indices.
- Unique to cubic crystals
  - Planes & directions having the same indices are perpendicular to one another
Crystallographic Planes

example

1. Intercepts  
   \[ \begin{array}{ccc} 
   a & b & c \\
   1 & 1 & \infty \\
   \end{array} \]

2. Reciprocals  
   \[ \begin{array}{ccc} 
   1/1 & 1/1 & 1/\infty \\
   1 & 1 & 0 \\
   \end{array} \]

3. Reduction  
   \[ \begin{array}{ccc} 
   1 & 1 & 0 \\
   \end{array} \]

4. Miller Indices  
   (110)

example

1. Intercepts  
   \[ \begin{array}{ccc} 
   a & b & c \\
   1/2 & \infty & \infty \\
   \end{array} \]

2. Reciprocals  
   \[ \begin{array}{ccc} 
   1/2 & 1/\infty & 1/\infty \\
   2 & 0 & 0 \\
   \end{array} \]

3. Reduction  
   \[ \begin{array}{ccc} 
   1 & 0 & 0 \\
   \end{array} \]

4. Miller Indices  
   (100)
Crystallographic Planes

**example**

1. **Intercepts**
   - 1/2  1  3/4

2. **Reciprocals**
   - 1/½  1/1  1/¾

3. **Reduction**
   - 6  3  4

4. **Miller Indices** (634)

**Family of Planes** \{hkl\}

**Ex:** \{100\} = (100), (010), (001), (100), (010), (001)
Determine the Miller indices for the plane shown in the sketch

![Diagram showing a crystal lattice with a plane highlighted.](image)

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>c/a</td>
<td>-b</td>
<td>c/2</td>
</tr>
<tr>
<td>(\infty)</td>
<td>-1</td>
<td>1/2</td>
</tr>
<tr>
<td>0</td>
<td>-1</td>
<td>2</td>
</tr>
</tbody>
</table>

Intercepts
- Intercept in terms of lattice parameters
- Reciprocals
- Reductions
- Enclosure

\((012)\) Plane
Crystallographic Planes (HCP)

- In hexagonal unit cells the same idea is used

<table>
<thead>
<tr>
<th>Example</th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$a_3$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Intercepts</td>
<td>1</td>
<td>$\infty$</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>2. Reciprocals</td>
<td>1</td>
<td>$1/\infty$</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>0</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>3. Reduction</td>
<td>1</td>
<td>0</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>4. Miller-Bravais Indices</td>
<td>(1011)</td>
<td></td>
<td></td>
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</tbody>
</table>

Adapted from Fig. 3.8(a), Callister 7e.
Figure 3.9 Representations of a series each of (a) (001), (b) (110), and (c) (111) crystallographic planes.
Example 3.11

- Construct a \((0\bar{1}1)\) plane within a cubic unit cell.
Atomic Arrangements

**Figure 3.10** (a) Reduced-sphere FCC unit cell with (110) plane. (b) Atomic packing of an FCC (110) plane. Corresponding atom positions from (a) are indicated.

**Figure 3.11** (a) Reduced-sphere BCC unit cell with (110) plane. (b) Atomic packing of a BCC (110) plane. Corresponding atom positions from (a) are indicated.
3.10 Crystallographic Planes

• Equivalent planes
  – Have the same atomic packing
  – Can be grouped into a family of planes

• Cubic crystals
  – \((111), (\bar{1} \bar{1} \bar{1}), (\bar{1} 11), (1 \bar{1} 1), ...\) are equivalent
  – Grouped together into the family: \(\{111\}\)
3.11 Linear and Planar Densities

- Equivalent directions have identical linear density
  \[
  LD = \frac{\text{# of atoms centered on direction vector}}{\text{length of direction vector}}
  \]

- Equivalent planes have identical planar density
  \[
  PD = \frac{\text{# of atoms centered on a plane}}{\text{area of plane}}
  \]
3.11 Linear and Planar Densities

Figure 3.12  (a) Reduced-sphere FCC unit cell with the [110] direction indicated. (b) The bottom face-plane of the FCC unit cell in (a) on which is shown the atomic spacing in the [110] direction, through atoms labeled X, Y, and Z.

\[ LD_{110} = \frac{\text{# atoms centered on direction vector} (\text{linear} \Rightarrow \text{atomic diameter represents atom})}{\text{length of direction vector}} \]

\[ = \frac{2}{4R} = \frac{1}{2R} \]
3.11 Linear and Planar Densities

\[ PD_{110} = \frac{\# \text{ of atoms centered on a plane (planar } \Rightarrow \text{ circular area represents atom)}}{\text{area of plane}} \]

\[ = \frac{2}{8R^2 \sqrt{2}} = \frac{1}{4R^2 \sqrt{2}} \]

**Figure 3.10** (a) Reduced-sphere FCC unit cell with (110) plane. (b) Atomic packing of an FCC (110) plane. Corresponding atom positions from (a) are indicated.
Linear Density for BCC

\[ \alpha = \frac{4R}{\sqrt{3}} \]

Calculate the linear density for the following directions:

a. [100]

b. [110]

c. [111]
Planar Density for BCC

\[ \alpha = \frac{4R}{\sqrt{3}} \]

Calculate the planar density for the following BCC planes:

a. (100)

b. (110)
3.12 Close-Packed Crystal Structure

- Close-packed directions
  - Directions with maximum atom-packing density
- Close-packed planes
  - Planes with maximum atom-packing density
- Atoms packed together are close-packed if they occupy the minimum volume possible (assuming they are incompressible spheres). They would have the maximum possible packing efficiency, defined as the ratio of volume of atoms to volume of space used.
3.12 Close-Packed Crystal Structures

FCC structures
- APF = 0.74
- CN = 12
- close-packed planes
- close-packed directions

HCP structures
- APF = 0.74
- CN = 12
- close-packed planes
- close-packed directions
3.12 Close-Packed Crystal Structures

3.12 Close-Packed Crystal Structures


Centers of this layer are directly above the bottom A layer.
3.12 Close-Packed Crystal Structures

Figure 3.13  (a) A portion of a close-packed plane of atoms; A, B, and C positions are indicated. (b) The AB stacking sequence for close-packed atomic planes. (Adapted from W. G. Moffatt, G. W. Pearsall, and J. Wulff, The Structure and Properties of Materials, Vol. I, Structure, p. 50. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)
Centers of this layer are above the C sites of the bottom A layer.

**Figure 3.15** (a) Close-packed stacking sequence for face-centered cubic. (b) A corner has been removed to show the relation between the stacking of close-packed planes of atoms and the FCC crystal structure; the heavy triangle outlines a (111) plane. (Figure b from W. G. Moffatt, G. W. Pearsall, and J. Wulff, *The Structure and Properties of Materials*, Vol. I, *Structure*, p. 51. Copyright © 1964 by John Wiley & Sons, New York. Reprinted by permission of John Wiley & Sons, Inc.)
3.12 Close-Packed Crystal Structures

FCC structures
• stacking sequence of the close-packed planes is ABCABC…

HCP structures
• stacking sequence of the close-packed planes is ABAB…
3.12 Close-Packed Crystal Structures

FCC structures

- stacking sequence of the close-packed planes is ABCABC…

HCP structures

- stacking sequence of the close-packed planes is ABAB…
3.13 Single Crystals

- Single crystal
  - the periodic & repeated arrangement of atoms is perfect or extends throughout the material without interruption.
  - Silicon single crystals in the semiconductor industry.
3.14 Polycrystalline Materials

- Polycrystalline
  - Composed of a collection of many crystals or grains
Figure 3.17  Schematic diagrams of the various stages in the solidification of a polycrystalline material; the square grids depict unit cells. (a) Small crystallite nuclei. (b) Growth of the crystallites; the obstruction of some grains that are adjacent to one another is also shown. (c) Upon completion of solidification, grains having irregular shapes have formed. (d) The grain structure as it would appear under the microscope; dark lines are the grain boundaries. (Adapted from W. Rosenhain, An Introduction to the Study of Physical Metallurgy, 2nd edition, Constable & Company Ltd., London, 1915.)
3.15 Anisotropy

- Anisotropy
  - Materials having different properties in different directions

- Isotropy
  - Materials having same properties in all directions.
## Anisotropy & Isotropy

### Table 3.3  Modulus of Elasticity Values for Several Metals at Various Crystallographic Orientations

<table>
<thead>
<tr>
<th>Metal</th>
<th>Modulus of Elasticity (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[100]</td>
</tr>
<tr>
<td>Aluminum</td>
<td>63.7</td>
</tr>
<tr>
<td>Copper</td>
<td>66.7</td>
</tr>
<tr>
<td>Iron</td>
<td>125.0</td>
</tr>
<tr>
<td>Tungsten</td>
<td>384.6</td>
</tr>
</tbody>
</table>

3.17 Non-crystalline Solids

- Non-crystalline materials (amorphous materials)
  - Do not have long-range order
  - May have short-range order

- Rapid cooling through the freezing temperature favors formation of a non-crystalline solid
  - Little time is allowed for the ordering process
3.17 Non-crystalline Solids

**Figure 3.18** Two-dimensional schemes of the structure of (a) crystalline silicon dioxide and (b) noncrystalline silicon dioxide.
Crystalline Solids

- **Metals**
  - Normally form crystalline solids
- **Ceramics**
  - Crystalline or amorphous
- **Polymers**
  - Non-crystalline or semi-crystalline

Increasing Tendency to Form Crystalline Solids