Chapter 3: Fundamentals of Crystallography

ISSUES TO ADDRESS...

• What is the difference in atomic arrangement between crystalline and noncrystalline solids?

• How are crystallographic directions and planes named?

• Under what circumstances does a material property vary with the measurement direction?
Energy and Packing

- Non dense, random packing

- Dense, ordered packing

Dense, ordered packed structures tend to have lower energies.
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
= Vitreous = Glassy

Adapted from Fig. 3.23(b), Callister & Rethwisch 8e.
Adapted from Fig. 3.23(a), Callister & Rethwisch 8e.
Crystal Systems

Unit cell: smallest repetitive volume which contains the complete lattice pattern of a crystal.

7 crystal systems

14 crystal lattices

\[ a, b, \text{ and } c \] are the lattice constants
<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><img src="image" alt="Cubic Unit Cell" /></td>
</tr>
<tr>
<td>Hexagonal</td>
<td>$a = b \neq c$</td>
<td>$\alpha = \beta = 90^\circ, \gamma = 120^\circ$</td>
<td><img src="image" alt="Hexagonal Unit Cell" /></td>
</tr>
<tr>
<td>Tetragonal</td>
<td>$a = b \neq c$</td>
<td>$\alpha = \beta = \gamma = 90^\circ$</td>
<td><img src="image" alt="Tetragonal Unit Cell" /></td>
</tr>
<tr>
<td>Rhombohedral (Trigonal)</td>
<td>$a = b = c$</td>
<td>$\alpha = \beta = \gamma \neq 90^\circ$</td>
<td><img src="image" alt="Rhombohedral Unit Cell" /></td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>$a \neq b \neq c$</td>
<td>$\alpha = \beta = \gamma = 90^\circ$</td>
<td><img src="image" alt="Orthorhombic Unit Cell" /></td>
</tr>
<tr>
<td>Monoclinic</td>
<td>$a \neq b \neq c$</td>
<td>$\alpha = \gamma = 90^\circ \neq \beta$</td>
<td><img src="image" alt="Monoclinic Unit Cell" /></td>
</tr>
<tr>
<td>Triclinic</td>
<td>$a \neq b \neq c$</td>
<td>$\alpha \neq \beta \neq \gamma \neq 90^\circ$</td>
<td><img src="image" alt="Triclinic Unit Cell" /></td>
</tr>
</tbody>
</table>
Point Coordinates

Point coordinates for unit cell center are
\[ \frac{a}{2}, \frac{b}{2}, \frac{c}{2} \]
\[ \frac{1}{2} \frac{1}{2} \frac{1}{2} \]

Point coordinates for unit cell corner are 111

Translation: integer multiple of lattice constants \(\rightarrow\) identical position in another unit cell
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 \( a, b, \) and \( c \):
   \[
   \frac{x_2 - x_1}{a} \quad \frac{y_2 - y_1}{b} \quad \frac{z_2 - z_1}{c}
   \]
4. Adjust to smallest integer values
5. Enclose in square brackets, no commas

\[
[uvw]
\]

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

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

=> 1, 0, 1/2  => 2, 0, 1

=> [201]
Crystallographic Directions

\[
\begin{align*}
[011] \\
[111] \\
[100] \\
[110]
\end{align*}
\]
Crystallographic Directions

Example 2:

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

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

\[
\begin{array}{ccc}
-a - a & b - b/2 & c - 0 \\
\hline
a & b & c
\end{array}
\]

=> -2, 1/2, 1

Multiplying by 2 to eliminate the fraction

-4, 1, 2 => [\overline{412}] where the overbar represents a negative index

families of directions <uvw>
Determination of HCP Crystallographic Directions

Algorithm

1. Determine coordinates of vector tail, pt. 1: \( x_1, y_1, \) \& \( z_1; \) and vector head, pt. 2: \( x_2, y_2, \) \& \( z_2. \)
in terms of three axis \((a_1, a_2, \text{and } z)\)
2. Tail point coordinates subtracted from head
point coordinates and normalized by unit cell
dimensions \( a \) and \( c \)
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas,
for three-axis coordinates \([u'v'w']\)
5. Convert to four-axis Miller-Bravais lattice
coordinates using equations below:
\[
\begin{align*}
    u &= \frac{1}{3} (2u' - v') \\
    v &= \frac{1}{3} (2v' - u') \\
    t &= -(u + v) \\
    w &= w'
\end{align*}
\]
6. Adjust to smallest integer values and
enclose in brackets \([uvtw]\)
Determination of HCP Crystallographic Directions

Determine indices for green vector

Example

<table>
<thead>
<tr>
<th></th>
<th>$a_1$</th>
<th>$a_2$</th>
<th>$z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Tail location</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>Head location</td>
<td>$a$</td>
<td>$a$</td>
</tr>
<tr>
<td>2. Normalized</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>3. Reduction</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>4. Brackets</td>
<td>[110]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5. Convert to 4-axis parameters</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
\begin{align*}
  u &= \frac{1}{3} \left[ (2)(1) - (1) \right] = \frac{1}{3} \\
  v &= \frac{1}{3} \left[ (2)(1) - (1) \right] = \frac{1}{3} \\
  t &= -\left( \frac{1}{3} + \frac{1}{3} \right) = -\frac{2}{3} \\
  w &= 0
\end{align*}
\]

6. Reduction & Brackets

$1/3, 1/3, -2/3, 0 \quad \Rightarrow \quad 1, 1, -2, 0 \quad \Rightarrow \quad [11\bar{2}0]$
Crystallographic Planes

Adapted from Fig. 3.7, *Callister & Rethwisch 9e.*
Crystallographic Planes

- **Miller Indices**: Reciprocals of the (three) axial intercepts for a plane, cleared of fractions & common multiples. All parallel planes have same Miller indices.

- **Algorithm**
  1. Read off intercepts of plane with axes in terms of $a$, $b$, $c$
  2. Take reciprocals of intercepts
  3. Reduce to smallest integer values
  4. Enclose in parentheses, no commas i.e., $(hkl)$
## Crystallographic Planes

**example**

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Intercepts</td>
<td>1</td>
<td>1</td>
<td>$\infty$</td>
</tr>
<tr>
<td>2. Reciprocals</td>
<td>$1/1$</td>
<td>$1/1$</td>
<td>$1/\infty$</td>
</tr>
<tr>
<td>3. Reduction</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>4. Miller Indices</td>
<td>(110)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**example**

<table>
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<tr>
<th></th>
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<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Intercepts</td>
<td>$1/2$</td>
<td>$\infty$</td>
<td>$\infty$</td>
</tr>
<tr>
<td>2. Reciprocals</td>
<td>$1/\frac{1}{2}$</td>
<td>$1/\infty$</td>
<td>$1/\infty$</td>
</tr>
<tr>
<td>3. Reduction</td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4. Miller Indices</td>
<td>(100)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Crystallographic Planes

example  \( a \quad b \quad c \)
1. Intercepts  \( 1/2 \quad 1 \quad 3/4 \)
2. Reciprocals  \( 1/\frac{1}{2} \quad 1/1 \quad 1/\frac{3}{4} \)
   \( 2 \quad 1 \quad 4/3 \)
3. Reduction  \( 6 \quad 3 \quad 4 \)
4. Miller Indices  \( (634) \)

Family of Planes  \( \{hkl\} \)

Ex:  \( \{100\} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1}) \)
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>
<td></td>
</tr>
</tbody>
</table>

Adapted from Fig. 3.8, Callister & Rethwisch 9e.
Crystallographic Planes (HCP)
Single Crystalline vs. Polycrystalline

Fig. 03.09

Photograph courtesy of irocks.com, Megan Foreman photo.

Fig. 03.10

Single Crystalline vs. Polycrystalline
Summary

• Atoms may assemble into **crystalline** or **amorphous** structures.

• **Crystallographic points, directions and planes** are specified in terms of indexing schemes. Crystallographic directions and planes are related to **atomic linear densities** and **planar densities**.

• Materials can be **single crystals** or **polycrystalline**. Material properties generally vary with single crystal orientation (i.e., they are **anisotropic**), but are generally non-directional (i.e., they are **isotropic**) in polycrystals with randomly oriented grains.