Class Exercise

- Draw the unit cell structure for simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) lattices.
- Give coordination number (CN) for atoms in each of those structures.
- Give the “average” number of atoms in a unit cell for simple cubic, body-centered cubic, and face-centered cubic structures and explain why.
Three Types of Unit Cell Structures for Cubic Crystal Systems

- **Simple**
  - \( n = 1 \)
  - \( a_1 \cdot a_2 \cdot a_3 = a^3 \)
  - \( \text{CN} = 6 \)

- **Body-Centered**
  - \( n = 2 \)
  - \( \text{CN} = 8 \)

- **Face-Centered**
  - \( n = 4 \)
  - \( \text{CN} = 12 \)

http://mysite.du.edu/~jcalvert/phys/lattice.htm
Class Exercise

Using the concepts for lattice and unit cell, for 2D lattices (of the same atoms) given below, please draw the 2D unit cell and determine the coordination number (CN) and number of atoms per unit cell (n).

CN (number of nearest neighbors) = 4
Average number of atoms per unit cell = 4 \times \frac{1}{4} = 1
(The dashed square in blue represents symmetry, but it is not the smallest)
(The dotted square in green is smallest, but does not represent symmetry: it can rotate any degree and does not distinguish from other patterns as on the right)
Polymorphism

- Two or more distinct crystal structures for the same material (allotropy/polymorphism) in terms of composition

<table>
<thead>
<tr>
<th>Phase</th>
<th>Temperature</th>
<th>Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>liquid</td>
<td></td>
<td></td>
</tr>
<tr>
<td>BCC</td>
<td>1538°C</td>
<td>δ-Fe</td>
</tr>
<tr>
<td>FCC</td>
<td>1394°C</td>
<td>γ-Fe</td>
</tr>
<tr>
<td>BCC</td>
<td>912°C</td>
<td>α-Fe</td>
</tr>
</tbody>
</table>
Virtual Materials Science & Engineering (VMSE)

• VMSE is a tool to visualize materials science topics such as crystallography and polymer structures in three dimensions
  
  • Available in Student Companion Site at http://www.wiley.com/college/callister/CL_EWSTU01031_S/vmse/
Unit Cells

- VMSE allows you to view the unit cells and manipulate them in three dimensions

- Below are examples of actual VMSE screen shots

![FCC Structure](image1.png) ![HCP Structure](image2.png)
Other Links

• Flash 3D Atomic Structure Model Viewer
  http://www.dawgsdk.org/crystal/index.en
Crystal Structure Application Problem 2
Estimation of Theoretical Density or Atom Size

Density = \( \rho = \frac{\text{Total mass of atoms in a unit cell}}{\text{Total volume of a unit cell}} \)

For simple pure element, if known:
- \( n = \text{number of atoms/unit cell} \)
- \( A = \text{atomic weight (in g/mol)} \)
- \( V_C = \text{Volume of unit cell, } V_c = a^3 \text{ for cubic structure} \)
- \( N_A = \text{Avogadro’s number} = 6.022 \times 10^{23} \text{ atoms/mol} \)

\[
\rho = \frac{n \left( \frac{A}{N_A} \right)}{V_C}
\]
Crystal Structure Application Problem 2

Estimation of Theoretical Density or Atom Size

- Ex: Cr (BCC unit cell)

Atom mass: \( A = 52.00 \text{ g/mol} \)

Atom radius: \( R = 0.125 \text{ nm} \)

\( n = 2 \text{ atoms/unit cell} \)

\[ a = 4 \frac{R}{\sqrt{3}} = 0.2887 \text{ nm} \]

\[ \rho_{\text{theoretical}} = 7.18 \text{ g/cm}^3 \]

\[ \rho_{\text{measured}} = 7.19 \text{ g/cm}^3 \]
Point Coordinates in Crystal Structure

- **Unit cell** – repeating unit that reflects crystal symmetry
- **Point coordinates:**
  - Specified in terms of its coordinates (fractional length in “projection”) with respect to the three edges of the unit cell,
  - Example:
    - Point P, with $q$ reflecting the projection of the point to $x$ axis, $r$ reflecting projection to $y$ axis, and $s$ reflecting project onto $z$ axis ($x$, $y$, $z$ axis along $a$, $b$, $c$ edge of the unit cell, with unit length of $a$, $b$, $c$, respectively), coordinate of $qrs$
- Axes may or may not be orthogonal to each other
- In some cases, some points are (geometrically) equivalent
Class Exercise – Coordinates of Points

• Specify the coordinates for three points as labeled in the graph for a (simple) cubic unit cell
  P  \( \frac{1}{2} \) 0  1
  Q  1  1  \( \frac{1}{2} \)
  R  0  1  1

• Label the points based on the coordinates given for a cubic unit cell
  P’  1  0  0
  Q’  \( \frac{1}{2} \)  \( \frac{1}{2} \)  0
  R’  0  0  \( \frac{1}{2} \)
Directions in Crystal Structure

1. Vector repositioned (if necessary) with starting point to pass through origin $O$.
2. Read off projections of the end point of the vector in terms of unit cell dimensions $a$, $b$, and $c$.
3. Adjust to smallest integer values.

Ex: $1, 0, \frac{1}{2} \rightarrow 2, 0, 1 \rightarrow [201]$ direction

$\frac{1}{2}, 1, \frac{1}{2} \rightarrow 1, 2, 1 \rightarrow [121]$ direction

$-1, 1, \frac{1}{2} \rightarrow -2, 2, 1 \rightarrow [\bar{2}21]$ direction

Overbar represents a negative index.

For some crystal systems, some directions are equivalent → families of directions, designated in the form of $<uvw>$.

e.g., for simple cubic, $[100]$, $[010]$, $[001]$, $[100]$, $[010]$, $[001]$ directions are all equivalent, as $<100>$ family.
Class Exercise – Directional Indices

• Specify the directional indices for the crystallography directions as labeled in the graph
  
  \[ v_1 [102] \]
  \[ v_2 [110] \]
  \[ v_3 [\overline{2}01] \]

• Draw the crystallography directions based on directional indices given below
  
  \[ v_4 [100] \]
  \[ v_5 [112] \]
  \[ v_6 [111] \]
Planes in Crystal Structure (1)

Adapted from Fig. 3.10, *Callister & Rethwisch 8e.*
Planes in Crystal Structure (2)

- **Miller Indices**: Indices given to describe crystal planes - Reciprocals of the (three) axial intercepts for a plane, cleared of fractions

- **Method**
  1. *If a crystal plane not passing through origin*, read off the intercepts of that plane with three axes of the unit cell in terms of edge length $a$, $b$, $c$ (*Otherwise a parallel plane or alternative origin has to be chosen so that the plane does NOT pass through the origin*)
  2. Take reciprocals for each of the three intercepts, respectively
  3. If contains non-integer, reduce to smallest integer set by multiplying a common integer, when applicable
  4. Enclose in parentheses, no commas i.e., $(hkl)$
Planes in Crystal Structure (4)

example

<table>
<thead>
<tr>
<th>Intercepts</th>
<th>1a</th>
<th>1b</th>
<th>(\infty)c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reciprocals</td>
<td>1/1</td>
<td>1/1</td>
<td>1/(\infty)</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

3. Miller Indices (110)

example

<table>
<thead>
<tr>
<th>Intercepts</th>
<th>1/2a</th>
<th>(\infty)b</th>
<th>(\infty)c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reciprocals</td>
<td>1/2</td>
<td>1/(\infty)</td>
<td>1/(\infty)</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

3. Miller Indices (200)

DO NOT reduce to (100)
**Planes in Crystal Structure (5)**

**example**

1. **Intercepts**
   - $x = 1/2a$
   - $y = 1b$
   - $z = 3/4c$

2. **Reciprocals**
   - $x = 1/\frac{1}{2}$
   - $y = 1/1$
   - $z = 1/\frac{3}{4}$

3. Multiply integer of 3
   - $x = 6$
   - $y = 3$
   - $z = 4$

4. **Miller Indices** (634)

For some crystal systems, some planes are equivalent

**Family of Planes** \{**hkl**\}. For example

**Cubic:** \{100\} family includes (100), (010), (001), (100), (010), (001) planes
Class Exercise (5) – Plane Miller Indices

• Specify the Miller indices for the crystallography planes as labeled in the graph

Axis $x \quad y \quad z$
Intercepts $a \quad a \quad \frac{1}{2}a$
Reciprocal $1 \quad 1 \quad 2$
Miller indices $(112)$

• Draw the crystallography $(122)$ plane

Miller indices $(122)$
Reciprocal $1 \quad \frac{1}{2} \quad \frac{1}{2}$
Axis $x \quad y \quad z$
Intercepts $a \quad \frac{1}{2}a \quad \frac{1}{2}a$
Class Exercise (6) – Plane Miller Indices

- Specify the Miller indices for the crystallography planes as labeled in the graph

<table>
<thead>
<tr>
<th>Axis</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intercepts</td>
<td>½a</td>
<td>½a</td>
<td>∞</td>
</tr>
<tr>
<td>Reciprocal</td>
<td>2</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>Miller indices</td>
<td>(220)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Draw the crystallography (101) plane

<table>
<thead>
<tr>
<th>Axis</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intercepts</td>
<td>a</td>
<td>∞</td>
<td>a</td>
</tr>
<tr>
<td>Miller indices</td>
<td>(101)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reciprocal</td>
<td>1</td>
<td>∞</td>
<td>1</td>
</tr>
</tbody>
</table>