Crystalline Solids with Cubic Unit Cells
Lab Experiment

Observe models & inspect solids with cubic unit cells

**Square Array Unit Cells:**
- general: simple cubic & bcc
- CsCl
- NaTl
- nitinol

**Close Packed Unit Cells:**
- general: ccp & fcc
- NaCl
- CaTiO$_3$
- YBa$_2$Cu$_3$O$_7$ superconductor
Amorphous or Crystalline?

The arrangement of the atoms, ions, or molecules making up a solid determine if that solid is amorphous or crystalline.

<table>
<thead>
<tr>
<th>“Atom” Arrangement</th>
<th>Amorphous</th>
<th>Crystalline</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symmetry?</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Packing</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

What qualitative observations provide a clue to which class a solid belongs to?
Terms & Definitions

Match the term to the definition.

1. Lattice
   A. smallest 3D repeat unit of a cell

2. Unit Cell
   B. # of lattice pts @ a lattice pt of interest

3. Lattice Points
   C. atoms/ions/molecules that are a solid’s framework

4. Coordination Number
   D. 3D system created by unit cells & lattice pts
Packing

What type of 2D packing is shown?

What is packing efficiency? Which type of packing above will result in higher packing efficiency?
Packing Order

- Layering of 2D arrays
- ABCs of Packing Order?

Scenarios: Provide the packing order:
- Layer 2 directly overlays Layer 1.
- Layer 2 overlays the holes of Layer 1.
- Layer 3 overlays the holes of Layer 2, which overlays the holes of Layer 1.
## Unit Cells

- Connect all related terms & pictures

<table>
<thead>
<tr>
<th>2D Arrays</th>
<th>Unit Cells</th>
<th>Pictures</th>
</tr>
</thead>
<tbody>
<tr>
<td>close packed</td>
<td>face centered cubic</td>
<td><img src="image1.png" alt="Picture" /></td>
</tr>
<tr>
<td>simple cubic</td>
<td><img src="image2.png" alt="Picture" /></td>
<td></td>
</tr>
<tr>
<td>square</td>
<td>hexagonal</td>
<td><img src="image3.png" alt="Picture" /></td>
</tr>
<tr>
<td></td>
<td>body centered cubic</td>
<td><img src="image4.png" alt="Picture" /></td>
</tr>
</tbody>
</table>
# lattice pts / unit cell

<table>
<thead>
<tr>
<th>Atom’s Position</th>
<th>Image</th>
<th>Cubic cells sharing atom, fract in 1 cell</th>
<th>Hex. cells sharing atom, fract in 1 cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corner</td>
<td><img src="image" alt="Corner Cubic" /></td>
<td><img src="image" alt="Corner Cubic" /></td>
<td><img src="image" alt="Corner Hexagonal" /></td>
</tr>
<tr>
<td>Edge</td>
<td><img src="image" alt="Edge Cubic" /></td>
<td><img src="image" alt="Edge Cubic" /></td>
<td><img src="image" alt="Edge Hexagonal" /></td>
</tr>
<tr>
<td>Face</td>
<td><img src="image" alt="Face Cubic" /></td>
<td><img src="image" alt="Face Cubic" /></td>
<td><img src="image" alt="Face Hexagonal" /></td>
</tr>
<tr>
<td>Internal</td>
<td><img src="image" alt="Internal Cubic" /></td>
<td><img src="image" alt="Internal Cubic" /></td>
<td><img src="image" alt="Internal Hexagonal" /></td>
</tr>
</tbody>
</table>
Simple Cubic Unit Cell

- Packing Order:

- # atoms / unit cell:

- Atoms touch:

- Coordination #:
Body Ctr’d d Cubic Unit Cell

- Packing Order:

- # atoms / unit cell:

- Atoms touch:

- Coordination #:
Hexagonal Unit Cell

- Packing Order:

- # atoms / unit cell:

- Atoms touch:

- Coordination #: 
Face Ctr’d Cubic Unit Cell

Cubic Close-Packing (ccp)

- Packing Order: A-B-C
Face Ctr’d d Cubic Unit Cell
(cont.)

**ROTATE 45°**
Face Ctr’d Cubic Unit Cell (cont.)

- # atoms / unit cell:

- Atoms touch:

- Coordination #:
Pythagorean’s Theorem & Cubic Unit Cells

\[ f^2 = e^2 + e^2 \]

\[ b^2 = f^2 + e^2 \]

Simplification:

Simplification:
Cubic Unit Cell Calculations

Determine the edge \( e \) of a body ctr’d cubic (bcc) unit cell as a function of radius \( r \).
Silver (Ag),

\[ r = 144 \text{ pm} \]
crystallizes in a ccp structure. Calculate Ag’s density.
## Summary of Unit Cells

<table>
<thead>
<tr>
<th>Type of Unit Cell</th>
<th>Image of Unit Cell</th>
<th>Packing Order</th>
<th># of atoms / cell</th>
<th>Where do spheres touch?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple (Primitive) Cubic</td>
<td><img src="image1" alt="Image" /></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Body Centered Cubic (bcc)</td>
<td><img src="image2" alt="Image" /></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hexagonal Close Packed (hcp)</td>
<td><img src="image3" alt="Image" /></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cubic Close Packed (ccp) Face</td>
<td><img src="image4" alt="Image" /></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Face Centered Cubic (fcc)</td>
<td><img src="image5" alt="Image" /></td>
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<td></td>
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</tr>
</tbody>
</table>

- **Simple (Primitive) Cubic**: Packing order and # of atoms/cell not specified. Spheres touch at vertices.
- **Body Centered Cubic (bcc)**: Packing order and # of atoms/cell not specified. Spheres touch at vertices.
- **Hexagonal Close Packed (hcp)**: Packing order and # of atoms/cell not specified. Spheres touch at vertices.
- **Cubic Close Packed (ccp) Face Centered Cubic (fcc)**: Packing order and # of atoms/cell not specified. Spheres touch at vertices.
Ionic Solids

- Larger ion (*usually anion*) = lattice points.
- Smaller ion (*usually cation*) sits in holes of lattice.
- Label each hole tetrahedral (t), octahedral (o), or cubic (c):
2 Ways to Determine an Ionic Cpd’s Empirical Formula

Ratio of # of ea ion w/i unit cell

Ratio of coord # of ea ion