7 Crystal Systems:
14 Bravais Lattices:

Additional Information:
See: Chapter 3

Unit Cells of the Bravais Lattices:

One of these has a mistake. Which one?
Crystal Structure is described by: Bravais lattice + basis (atoms decorating lattice point)

Also called: Space lattice + Motif

Examples of Crystal Structures: Diamond Cubic Lattice & Zinc Blende

FIGURE 3.7-4 (a) The diamond cubic crystal structure is composed of an FCC lattice with two atoms per lattice point. One atom from each pair is centered on each lattice point, and the second atom is positioned at (a0, 1/2, 1/2) and (a, 1/2, 1/2). (b) The zinc blende crystal structure is similar to the diamond cubic structure, except that the basis is composed of two different atoms.

Examples of: a) Si & Ge; b) ZnS, ZnSe, GaAs

Unit Cells of the Bravais Lattices:

Unit Cells are an array of lattice points in a specific Bravais lattice that, when periodically repeated, forms the entire lattice.

There are two types of unit cells:

- Conventional unit cell
  - Most geometrically convenient
  - 1 or more lattice points per unit cell

- Primitive unit cell
  - Smallest unit cell possible
  - Only one lattice point
**Fundamentals of Crystallography**

- **Examples of Primitive Unit Cells:**
  - FCC & BCC

  ![FCC & BCC Diagram](image)

  Blakemore, Solid State Physics 2nd Ed (Cambridge, 1985)

- **PEROVSKITES** - Example of:
  - Primitive Unit Cell
  - Crystal Structure = Bravais Lattices/space lattice + Basis

![Perovskite Diagram](image)

**Information**
- **Formula:** $\text{M}_x\text{M}_y\text{X}_z$
- **Bravais Lattice:** simple cubic
- **Basis:** 5 ions (1Ba$^{2+}$, 1Ti$^{4+}$, 3O$^{2-}$)
- **Atoms per Unit Cell:** 5

Shackelford, Intro to Materials Science for Engineers, 5th Ed. (Prentice Hall, 2002)
Crystallographic Directions: a crystallographic direction is defined as a line between 2 pts, or a vector. The following steps are utilized in the determination of the 3 directional indices:

- 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.
- The length of the vector projection on each of the 3 axes is determined; these are measured in terms of the unit cell dimensions \(a\), \(b\), and \(c\).
- These 3 numbers are multiplied or divided by a common factor to reduce them to the smallest integer values.
- The 3 indices (not separated by commas) are enclosed in square brackets:
  - \([uvw]\) where \(u\), \(v\), and \(w\) integers correspond to the reduced projection along the \(x\), \(y\), and \(z\) axes, respectively.

![Figure 3.5](image)

**Figure 3.5** The \([100]\), \([110]\), and \([111]\) directions within a unit cell.

Crystallographic Directions: an Example

**Example Problem 3.4**

Determine the indices for the direction shown in the accompanying figure.

**Solution**

The vector, as drawn, passes through the origin of the coordinate system, and therefore no translation is necessary. Projections of this vector onto the \(x\), \(y\), and \(z\) axes are, respectively, \(a/2\), \(b\), and \(6c\), which become \(1\), \(1\), and \(0\) in terms of the unit cell parameters (i.e., when the \(a\), \(b\), and \(c\) are dropped). Reduction of these numbers to the lowest set of integers is accomplished by multiplication of each by the factor 2. This yields the integers 1, 2, and 0, which are then enclosed in brackets as \([120]\).

This procedure may be summarized as follows:

<table>
<thead>
<tr>
<th>Projections (a/2)</th>
<th>Projections (in terms of (a), (b), and (c))</th>
<th>Reduction</th>
<th>Enclosure</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a/2)</td>
<td>(b)</td>
<td>1</td>
<td>([120])</td>
</tr>
<tr>
<td>(a/2)</td>
<td>(6c)</td>
<td>0</td>
<td>([120])</td>
</tr>
</tbody>
</table>

Fundamentals of Crystallography

Crystallographic Directions: an Example

What directions are the bonds in Si & Zinc Blende materials?

![Diagram of crystal structures]

Examples of: a) Si & Ge; b) ZnS, ZnSe, GaAs

Crystallographic Planes: Crystallographic planes in all but the hexagonal crystal system are specified by 3 Miller indices: (hkl). Any 2 planes parallel to each other are equivalent & have identical indices. The procedure used in determination of the h, k, and l Miller index numbers is as follows:

- If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell.
- At this point, the crystallographic plane either intersects or parallels each of the 3 axes; the length of the planar intercept for each axis is determined in terms of the lattice constants a, b, and c.
- The reciprocals of these numbers are taken. A plane that parallels an axis may be considered to have an infinite intercept, &, therefore, a zero index.
- If necessary, these 3 numbers are changed to the set of smallest integers by multiplication or division by a common factor.
- Finally, the integer indices (not separated by commas) are enclosed in parentheses: (hkl).
Crystallographic Planes: Several Examples

**Example Problem 3.6**

Determine the Miller indices for the plane shown in the accompanying sketch (a).

**Solution**

Since the plane passes through the selected origin O, a new origin must be chosen at the corner of an adjacent unit cell, taken as O' and shown in sketch (b). This plane is parallel to the z-axis, and the intercept may be taken as w = 0.

The y and z axes intercepts, referred to the new origin O', are -1 and w, respectively. Thus, in terms of the lattice parameters a, b, and c, these intercepts are \( w = -1 \), \( y = -1 \), and \( z = w \) since all are integers, no further reduction is necessary. Finally, reduction in parentheses yields \( \{100\} \).

These steps are briefly summarized below:

- **Intercepts**
  - \( w = -1 \)
  - \( y = -1 \)
  - \( z = w \)

- **Intercepts (in terms of lattice parameters)**
  - \( w = -1 \)
  - \( y = -1 \)
  - \( z = w \)

- **Reduction**
  - \( \{100\} \)


Family of planes

- Those planes which are equivalent in the crystal by symmetry
- Designated by \( \{ \} \)
- \( \{100\} = (100) + (010) + (001) + (-100) + (0-10) + (00-1) \)
Comparison of Packing of Atoms in the FCC & HCP Structures:

Stacking sequence in FCC Crystals for (111) planes:
ABCABC

FCC
HCP

Plane A
Or
A sites

Plane B
Or
B sites

Plane C
Or
C sites

Figure 14.2: The manner in which close-packed layers of spheres can be stacked to produce a variety of unit cell arrangements (left: hexagonal close-packed, HCP structure and right: face-centered cubic, FCC structure). After L. Pauling, The Nature of the Chemical Bond (Cornell, 1939).

Extra for those of you that are interested
Crystallographic Directions:

Example of the Hexagonal system:

\[ \mathbf{\hat{r}} = u\mathbf{\hat{a}}_1 + v\mathbf{\hat{a}}_2 + t\mathbf{\hat{a}}_3 + w\mathbf{\hat{c}} \]

where the direction is written:

\([uvw]\)

and the following condition imposed:

\[ u + v + t = 0 \]

Several Examples of the Hexagonal system:

Barrett & Massalski, Structure of Metals 3rd Ed (Pergamon, 1980)
Hexagonal Indices for Planes:

- To determine the indices for planes in the hexagonal crystal system, the 3 axes system used in the other crystal systems are not usually used because equivalent planes do not have similar indices.
- For this reason, it is preferable to use the four axes: \( a_1, a_2, a_3, c \)
- The Miller indices are: \((hkl)\)

where \(i=-(h+k)\) or \(h+k+i=0\)

<table>
<thead>
<tr>
<th>Example:</th>
<th>Axis:</th>
<th>(a_1)</th>
<th>(a_2)</th>
<th>(a_3)</th>
<th>(c)</th>
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<td>(-1/2)</td>
<td>(\infty)</td>
<td></td>
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<td>Reciprocal:</td>
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<td>0</td>
<td></td>
</tr>
<tr>
<td>Reduce:</td>
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<td>1</td>
<td>(-2)</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Miller Indices:</td>
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<td>1</td>
<td>(-2)</td>
<td>0</td>
<td></td>
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\[(1\underline{1}20)\text{ or (11.0)}\]

Determining Hexagonal Indices for Planes:

- If the plane passes through the selected origin, either another parallel plane must be constructed within the unit cell by an appropriate translation, or a new origin must be established at the corner of another unit cell.
- At this point, the crystallographic plane either intersects or parallels each of the 4 axes; the length of the planar intercept for each axis is determined in terms of the lattice constants \(a_1, a_2, a_3, c\).
- The reciprocals of these numbers are taken. A plane that parallels an axis may be considered to have an infinite intercept, \& therefore, a zero index.
- If necessary, these 3 numbers are changed to the set of smallest integers by multiplication or division by a common factor.

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</tbody>
</table>

\[(1\underline{1}20)\text{ or (11.0)}\]
Packing of Atoms in the FCC Structure:

- Structure: Face-centered cubic (fcc)
- Bravais lattice: fcc
- Atomic unit cell: $\frac{a}{2} \times \frac{a}{2} \times \frac{a}{2}$
- Typical metals: Fe, Al, Ni, Cu, Ag, Pb, and Au

Packing of Atoms in the BCC Structure:

- Structure: Body-centered cubic (bcc)
- Bravais lattice: bcc
- Atomic unit cell: $1 \times \frac{a}{2} \times \frac{a}{2}$
- Typical metals: Mo, Tl, Ga, In, Na, and W
Comparison of Packing of Atoms in the FCC & HCP Structures:

- **FCC**
  - Stacking of close-packed planes
  - Normal to close-packed planes
  - Face-centered cubic

- **HCP**
  - Stacking of close-packed planes
  - Normal to close-packed planes
  - Hexagonal close-packed

Figure 3.33: Comparison of the fcc and hcp structures. These are each efficient packings of close-packed planes. The difference between the two structures is the different stacking sequences. (After B. D. Cullity, Elements of X-Ray Diffraction, 2nd ed., Addison-Wesley Publishing Co., Inc., Reading, Mass., 1978.)

Blakemore, Solid State Physics 2nd Ed (Cambridge, 1985)

Packing of Atoms in the HCP Structure:

- **HCP**
  - Atom in unit cell
  - 2 atoms per lattice plane

- **FCC**
  - Atom centered in adjacent unit cell
  - One-twelfth of an atom

Figure 3.34: Hexagonal close-packed (hcp) structure for metals showing (a) the arrangement of atom centers relative to lattice points for a unit cell. These are two atoms per lattice point (note the outlined examples). (b) The actual packing of atoms within the unit cell. Note that the atom in the midplane extends beyond the unit cell boundaries. (c) The repeating hcp structure, equivalent to many adjacent unit cells (Part c courtesy of Molecular Simulations, Inc.).

Shackelford, Intro to Materials Science for Engineers, 5th Ed. (Prentice Hall, 2002)

Crystalline and Noncrystalline Materials:

**Question:** How would you calculate the density of a material given the:

- Lattice constant or Radius of Atom
- Crystal structure
- Atomic weight

where density is given by: \( \text{mass/volume} \)?

**Use Following Information:** Cu, FCC, \( r_{Cu} = 0.128 \) nm, Atomic Mass=63.5 g/mole.

Isotropic Materials:

- If the properties of the material are *independent* of the direction in which they are measured, the material is categorized as *isotropic*.

Anisotropy Materials:

- If the properties of the material are *dependent* of the direction in which they are measured, the material is categorized as *anisotropic*.

Examples of these properties include:

- Periodicity of atoms in a crystal structure.
- Density of a material of crystalline solids.
- Carrier velocity.
- Phonon velocity.
Crystalline and Noncrystalline Materials:

- **Allotropy:**
  - Elements that can exhibit more than one crystal structure are *allotropic*.

- **Polymorphism:**
  - Compounds that behave in the same manner as allotropic materials are referred to as *polymorphic*.

![Figure 3.10-1: A comparison of the polymorphs of carbon: (a) diamond and (b) graphite.](image)

Additional content:

- **Single Crystal:**
  - A continuous periodic crystal structure only interrupted by the boundaries of the solid.

- **Amorphous:**
  - Although short range periodicity may be present, long range periodicity is absent. Hence, amorphous material is not crystalline.

- **Polycrystalline:**
  - A material composed of from two to many single crystal grains.
\[
\begin{bmatrix}
1 & 2 & 1 \\
2 & -1 & -1 \\
1 & -2 & -1 \\
\end{bmatrix}
\]