Crystallographic directions and planes

Outline

• Crystallographic directions
• Crystallographic planes
• Linear and planar atomic densities
• Close-packed crystal structures
Point Coordinates

Point coordinates for unit cell center are

\[ \frac{a}{2}, \frac{b}{2}, \frac{c}{2} \quad \frac{1}{2} \frac{1}{2} \frac{1}{2} \]

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. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions \(a\), \(b\), and \(c\)
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas

\[ [uvw] \]

ex: \(1, 0, \frac{1}{2}\) => \(2, 0, 1\) => \([201]\)

\(-1, 1, 1\) => \([\bar{1}11]\) where overbar represents a negative index

families of directions \(<uvw>\)
Examples

Sketch the following directions: [110], [-1-21], [-1 0 2]
HCP Crystallographic Directions

Algorithm

1. Vector repositioned (if necessary) to pass through origin.
2. Read off projections in terms of unit cell dimensions $a_1$, $a_2$, $a_3$, or $c$
3. Adjust to smallest integer values
4. Enclose in square brackets, no commas

$[uvtw]$

ex: $\frac{1}{2}, \frac{1}{2}, -1, 0 \implies [1\bar{1}20]$

dashed red lines indicate projections onto $a_1$ and $a_2$ axes

Adapted from Fig. 3.8(a), Callister 7e.
HCP Crystallographic Directions

• Hexagonal Crystals
  – 4 parameter Miller-Bravais lattice coordinates are related to the direction indices (i.e., $u'v'w'$) as follows.

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

Fig. 3.8(a), Callister 7e.
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
Crystallographic Planes
Crystallographic planes (continued)

- Construct planes by Miller indices of planes (0 -1 -1) and (1 1 -2)
Chapter 3 -

Atomic arrangements

- The atomic arrangement for a crystallographic plane depends on the crystal structure

FCC: (a) reduced sphere (b) atomic packing of an FCC (110) plane

BCC: (a) reduced sphere (b) atomic packing of an BCC (110) plane
Atomic arrangements

• A family of planes contains all the planes that are crystallographically equivalent.

• In cubic system, planes with same indices, irrespective of order and sign, are equivalent
  – (111), (111), (111) ... belong to {111} family
  – (1100), (100), (010), and (001) belong to {100} family
  – (123), (123), (312) in cubic crystals belong to {123} family

• In tetragonal, (001) (001) are not as same family as (100), (100)
Linear and planar atomic density

- **Linear Density of Atoms** is defined as:
  \[
  \text{LD} = \frac{\text{Number of atoms}}{\text{Unit length of direction vector}}
  \]

- **Atomic planar density**: number of atoms centered on a plane/area of plane
  \[
  \text{Planar Density} = \frac{\#\text{atoms}}{\text{Area(2D repeat unit)}}
  \]
Planar Density of (100) Iron

Solution: At $T < 912^\circ C$ iron has the BCC structure.

Adapted from Fig. 3.2(c), Callister 7e.

2D repeat unit
Close-packed crystal structures

Close-packed plane stacking sequence for HCP

Close-packed plane stacking sequence for HCP