Lattice Geometry Identification

Crystallographic Planes and Directions
X-Ray Diffraction

Importance of Crystal Structures, Directions, Planes?

- Properties depend on geometry of crystals
  - Speed of light, sound
  - Strength
  - Conductivity
- In cubic single crystals properties are isotropic, all other systems are anisotropic
Crystallographic Planes & Directions

- Many material properties and processes vary with direction in the crystal.
- It is often necessary to be able to specify certain directions and planes in crystals.
- Directions and planes are described using three integers - Miller Indices.

Indexing in 2D

- Determine \( \Delta \) in unit distances to move from one lattice point to the next in the plane (or direction).
- Put in \( x,y \) format.

Properties:
- **Lowest Indices** - Greatest plane spacing
- **Lowest Indices** - Greatest density of lattice points

This is true in 3-D as well.
General Rules for Lattice Directions, Planes & Miller Indices

- Miller indices used to express lattice *planes* and *directions*
- $x, y, z$ are the axes (on arbitrarily positioned origin)
  - in some crystal systems these are not mutually $\perp$
- $a, b, c$ are lattice parameters (length of unit cell along a side)
- $h, k, l$ are the Miller indices for *planes* and *directions* - expressed as $(hkl)$ and $[hkl]$
Miller Indices for Directions

Recipe

- Draw vector, define tail as origin.
- Determine length in unit cell dimensions, a, b, and c.
- Remove fractions by multiplying by smallest possible factor.
- Enclose in square brackets.
- What is ???
  - $x = 1/2$, $y = 0$, $z = 1$
  - $[1/2 0 1] \rightarrow [1 0 2]$

Entire lattice can be referenced by one unit cell!

Example - Naming Directions
Example - Drawing Directions

- Draw \([112]\), \([\overline{1}1\overline{1}]\) and \([\overline{2}\overline{2}\overline{2}]\)

Families of Directions

- Equivalence of directions
  - e.g. \([123]\), \([213]\), \([312]\), \([132]\), \([231]\)
  - (only in a cubic crystal)
  - In the cubic system directions having the same indices regardless of order or sign are equivalent
Miller Indices for Planes

- (hkl) Crystallographic plane
- \{hkl\} Family of crystallographic planes
  - e.g. (hkl), (lhk), (hlk) etc.
  - In the cubic system planes having the same indices regardless of order or sign are equivalent
- Hexagonal crystals can be expressed in a four index system (u v t w)
  - Can be converted to a three index system using formulas

Recipe

- If the plane passes through the origin, select an equivalent plane or move the origin
- Determine the intersection of the plane with the axes in terms of a, b, and c
- Take the reciprocal \(1/\infty = 0\)
- Convert to smallest integers (optional)
- Enclose by parentheses

Note - plane // to axis, intercept = \(\infty\) and \(1/\infty = 0\)
Crystallographic Planes

X-Ray Diffraction
- Can be used to determine crystal structure (and hence identity of an unknown material)
- Diffraction occurs whenever a wave encounters a series of regularly spaced objects that:
  - Can scatter the wave
  - Have a spacing comparable to the wavelength
- X-ray wavelength \(\sim\) inter-atomic spacing and are scattered by atoms.
Constructive & Destructive Interference

Constructive
Maximum and minimum results from two diffracting beams phase shifted from one another.

Destructive

Bragg’s Law

- For constructive interference, the additional path length $SQ + QT$ must be an integral number of wavelengths: Real diffraction is more complicated for non-simple cubic

$$n\lambda = SQ + QT = d_{hkl}\sin\theta + d_{hkl}\sin\theta = 2d_{hkl}\sin\theta$$

$n = 1,2,3\ldots$ order of reflection

X-ray Source: Monochromatic and in-phase
Bragg’s Law, Cubic Symmetry

- Real diffraction is more complicated for non-simple cubic systems because some set’s of atoms (e.g. BCC center atoms) can produce out of phase scattering at certain Bragg angles $\theta$. Net effect...some of the diffracted beams, that according to Bragg’s Law should be present, are cancelled out.
- Example - for diffraction to occur:

| BCC | $h + k + l$ must be even |
| FCC | $h, k, l$ must all be either even or odd |

- Magnitude of difference between two adjacent and parallel planes of atoms is function of Miller Indices and the lattice parameter. For cubic symmetry:

$$d_{hkl} = \frac{a}{(h^2 + k^2 + l^2)^{1/2}}$$

Diffractometer Technique

- Use powder (or polycrystalline) sample to guarantee some particles will be oriented properly such that every possible set of crystallographic planes will be available for diffraction.

- Each material has a unique set of planar distances and extinctions, making X-ray diffraction useful in analysis of an unknown.
Example

- For BCC Fe, compute
  a) the interplanar spacing
  b) the diffraction angle for (220) set of planes.

  The lattice parameter for Fe is 0.2866 nm and the wavelength used is 0.1790 nm. Consider 1st order reflections only.

Reading Assignment

Shackelford 2001(5th Ed)
Read: pp 88, 101-110
Check class web site:
www.public.iastate.edu/~bastaw/courses/Mate271.html